BEST AVAILABLE RETROFIT TECHNOLOGY APPLICABILITY ANALYSIS
AIR QUALITY MODELING PROTOCOL
HONEYWELL ▪ HOPEWELL, VIRGINIA

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1. INTRODUCTION

Honeywell International Inc. operates a chemical manufacturing plant in Hopewell, Virginia. The Honeywell Hopewell plant is a major source of air emissions and submitted a Title V application on June 30, 1998, and is expected to receive a final Title V permit in the coming months. Currently, Honeywell is operating under air permit registration number 50232, issued by the Virginia Department of Environmental Quality (DEQ). The facility is considered eligible to be regulated under the Best Available Retrofit Technology (BART) provisions of the Regional Haze Rule.

The purpose of this document is to present the Honeywell Hopewell BART Applicability Protocol, due April 15, 2006. Air quality modeling will be used to determine whether the emissions from Honeywell's BART-eligible sources cause or contribute to visibility impairment at any federally protected Class I area, and hence whether a BART determination is necessary. This modeling protocol is presented to describe the procedures, analytical techniques, and data resources Honeywell proposes to use to make the applicability determination. Honeywell's evaluation of BART-eligibility and the proposed modeling methods to determine applicability of BART as described in this protocol are consistent with the following guidance documents:

- U.S. EPA, "Regional Haze Regulations and Guideline for Best Available Retrofit Technology (BART) Determinations," *Federal Register* Volume 70, Number 128, July 6, 2005.
- U.S. EPA, *Guidance for Tracking Progress under the Regional Haze Rule* (EPA-54/B-03-004), September 2003.
- U.S. EPA, *Guidance for Estimating Natural Visibility Conditions under the Regional Haze Rule* (EPA-454/B-03-005), October 2003.
- U.S. EPA, *Interagency Workgroup on Air Quality Modeling (IWAQM) Phase 2 Summary Report* (EPA-454/R-98-019), December 1998.
- U.S. EPA, *Guideline on Air Quality Models*, 40 CFR Part 51, Appendix W (Revised, November 9, 2005).
- VISTAS, *Protocol for the Application of the CALPUFF Model for Analyses of Best Available Retrofit Technology (BART), Revision 2*, March 9, 2006.
- VISTAS and U.S. EPA, "Q&A for Source by Source BART Rule" (Draft), October 28, 2005.
- Virginia DEQ BART Guidance, http://www.deq.state.va.us/air/bart.html

The *VISTAS BART Modeling Protocol* is incorporated by reference for Honeywell's source-specific modeling protocol, and is presented in Appendix A of this modeling protocol document. This BART applicability modeling protocol is submitted to DEQ to provide the opportunity for review and comment in conjunction with review by the U.S. EPA and Federal Land Managers (FLM) responsible for oversight of the federally-protected Class I areas potentially affected by Honeywell's Hopewell plant BART-eligible operations. As of the date of this protocol, certain modeling data resources have not yet been made available by VISTAS, as identified in this document. In addition to DEQ's review and comment on this protocol, Honeywell anticipates additional communication with DEQ throughout the BART implementation process as details become available during the time between this modeling protocol is submitted and Honeywell's BART Applicability Analysis is submitted to ensure that refined analyses (if required) are conducted using mutually agreeable data resources and processing options.

1.1 Overview of Regional Haze Rule and BART Requirements

The Regional Haze Rule requires that major sources of visibility-affecting pollutants belonging to one or more of 26 specific industrial source categories evaluate BART if the source was "in existence" (i.e., built or reconstructed) before August 7, 1977 and began operation after August 7, 1962. Such sources are termed "BART-eligible sources." Major sources of visibility-affecting pollutants have the potential to emit 250 tons per year (tpy) of one or more of oxides of nitrogen (NO_X), sulfur dioxide (SO_2), and particulate matter less than 10 micrometers in aerodynamic diameter (PM_{10}). Chemical process plants are one of the listed source categories, and include chemical manufacturing operations that are considered to be part of major SIC code "28" – Chemicals and Allied Products. Hereafter, the "BART-eligible source" is taken to mean the collection of sources at a facility in existence during the relevant time period within one or more BART source categories that has potential emissions of one or more visibility-affecting pollutants in excess of 250 tpy. The BART-eligible source may include multiple emission units but need not include the entire facility.

Industrial boilers greater than 250 million British thermal units per hour (MMBtu/hr) in heat input capacity are also considered a listed BART-eligible source category. However, the boiler at Honeywell's Hopewell plant (Boiler #8) began operation prior to 1962. Therefore, the boiler is not part of the BART-eligible source and was not considered in this BART analysis.

1.1.1 Determination of BART-eligibility

The U.S. EPA BART guidelines define the following three steps for determining which sources at a facility are BART-eligible:

1. Identify the emission units in the BART source categories.
2. Identify the start-up dates of those units.
3. Compare potential emissions to the 250 tpy cutoff.

Honeywell's Hopewell plant and DEQ have determined that ten emission units comprise the BART-eligible source because the units operate at a chemical plant, were in existence on August 7, 1977, and began operation after August 7, 1962.[1] This collection of ten emission units has potential emissions of greater than 250 tpy of NO_X, PM_{10}, and SO_2. Accordingly, the BART-eligible emission units at Honeywell's Hopewell plant will be evaluated to determine whether a BART determination is required or whether the facility can be considered exempt from BART. Specific information about these emission units is provided in Section 2 of this modeling protocol.

[1] Sources with no PM_{10}, NO_X, or SO_2 emissions as well as sources that are insignificant under the Title V operating permit program were exempted from consideration per DEQ's guidance.

1.1.2 ASSESSMENT OF CONTRIBUTION TO VISIBILITY IMPAIRMENT AND BART APPLICABILITY

In its role as technical analysis coordinator, VISTAS developed a common modeling protocol and data resources for use by state regulatory agencies and BART-eligible sources. The final *VISTAS BART Modeling Protocol* was issued on December 22, 2005, was revised most recently on March 9, 2006, and prescribes modeling techniques and data resources to conduct screening and refined analyses to assess whether a BART-eligible source is subject to BART.

A BART-eligible source is determined to be subject to BART if the source causes or contributes to visibility impairment at a federally protected Class I area. Causation is defined as a single-source impact of 1.0 deciviews (dv) or more; contribution is defined as a single-source impact of 0.5 dv or more (each evaluated on a 24-hour average basis). The deciview is a metric used to represent normalized light extinction attributable to visibility-affecting pollutants. To determine whether a BART-eligible facility causes or contributes to visibility impairment, U.S. EPA guidance requires the use of an air quality model, specifically recommending the CALPUFF modeling system, to quantify the impacts attributable to a single BART-eligible source. Because contribution to visibility impairment is sufficient cause to require a BART determination, 0.5 dv is the critical threshold for assessment of BART applicability.

Regional haze is measured using the light extinction coefficient (b_{ext}), which is expressed in terms of the haze index expressed in dv. The haze index (*HI*) is calculated as shown in the following equation.

$$HI = 10\ln\left(\frac{b_{ext}}{10}\right)$$

The impact of a BART-eligible source is determined by comparing *HI* for estimated natural background conditions with the impact of the source and without the impact of the source. The background extinction coefficient $b_{\text{ext, background}}$ is affected by various chemical species and the Rayleigh scattering phenomenon and can be calculated as shown in the following equation.

$$b_{ext,background}(km^{-1}) = b_{SO_4} + b_{NO_3} + b_{OC} + b_{soil} + b_{coarse} + b_{ap} + b_{ray}$$

where,

$b_{SO_4} = 0.003\,[(NH_4)_2SO_4]\,f(RH)$
$b_{NO_3} = 0.003\,[NH_4NO_3]\,f(RH)$
$b_{OC} = 0.004\,[OC]$
$b_{Soil} = 0.001\,[Soil]$
$b_{Coarse} = 0.0006\,[\text{Coarse Mass}]$
$b_{ap} = 0.01[\text{Elemental Carbon}]$
b_{Ray} = Rayleigh Scattering
f(RH) = relative humidity adjustment factor
[ ] = Concentration in $\mu g/m^3$

Values for the parameters listed above specific to the natural background conditions at the Class I areas considered in this analysis are provided on an annual average basis in the U.S. EPA's *Guidance for Estimating Natural Visibility Conditions Under the Regional Haze Rule*.[2] More detailed information about the natural background conditions particular to Class I areas potentially affected by Honeywell's operations at the Hopewell plant are provided in Section 3.5 of this protocol.

Particulate species that affect visibility are emitted from anthropogenic sources in various phases and include coarse particulate matter (PMC), fine particulate matter (PMF), secondary organic aerosols (SOA), and elemental carbon (EC), as well as precursors to fine particulate matter such as SO_2 and NO_X. Honeywell's calculation of speciated visibility affecting pollutant emissions is presented in Section 2 of this modeling protocol. The extinction coefficient due to emissions of visibility-affecting pollutants from a single BART-eligible source $b_{ext,source}$ is calculated using an air quality model. The extinction due to the BART-eligible source will be calculated as shown in the following equation.

$$b_{ext,source}(km^{-1}) = b_{SO_4} + b_{NO_3} + b_{PMC} + b_{PMF} + b_{SOA} + b_{EC}$$

where,

$b_{SO_4} = 0.003\,[(NH_4)_2SO_4]\,f(RH)$
$b_{NO_3} = 0.003\,[NH_4NO_3]\,f(RH)$
$b_{PMC} = 0.0006[PMC]$
$b_{PMF} = 0.001[PMF]$
$b_{soa} = 0.004[SOA]$
$b_{EC} = 0.01[EC]$
$f(RH)$ = relative humidity adjustment factor
[ ] = Concentration in $\mu g/m^3$

[2] U.S. EPA, *Guidance for Estimating Natural Visibility Conditions Under the Regional Haze Rule*, Table 2-1, Attachment A, September 2003, EPA-454/B-03-005.

Honeywell proposes to utilize screening modeling techniques, and if necessary, refined modeling techniques as described in the *VISTAS BART Modeling Protocol* to determine whether BART-eligible operations at the Hopewell plant contribute to visibility impairment at any Class I areas within 300 km. The CALPUFF modeling system will be used to compute the 24-hour average visibility impairment attributable to Honeywell and to assess whether the 0.5 dv contribution threshold is exceeded, and if so, the frequency, duration, and magnitude of any exceedance events. The U.S. EPA BART guidelines prescribe that the 98^{th} percentile, 24-hour average, visibility impact computed in a modeling analysis that evaluates three years of meteorological data should be compared to the contribution threshold. However, VISTAS prescribes that the *maximum* computed visibility impact be used as the basis for comparison in the screening analysis and the 98^{th} percentile impact in the refined analysis. To assess whether BART-eligible operations contribute to visibility impairment, Honeywell's applicability modeling analysis will quantify the top eight 24-hour average visibility impacts of each year modeled to illustrate the distribution (i.e., frequency, duration, and magnitude) of peak visibility impairment episodes attributable to the Hopewell plant.

CALPUFF is a refined air quality modeling system that is capable of simulating the dispersion, chemical transformation, and long-range transport of multiple visibility affecting pollutant emissions from a single source and is therefore preferred for BART applicability and determination analyses. The CALPUFF modeling system is described in technical detail in the *VISTAS BART Modeling Protocol* and its use in screening and refined analyses for BART applicability assessment of Honeywell's Hopewell plant is described in Sections 3, 4, and 5 of this modeling protocol.

The *VISTAS BART Modeling Protocol* specifies that all Class I areas within 300 km of a BART-eligible source must be initially evaluated to determine whether the source contributes to visibility impairment. Table 1-1 summarizes the distances separating Honeywell's Hopewell plant from all Class I areas within the VISTAS region and adjacent states. Consistent with the *VISTAS BART Modeling Protocol*, only those Class I areas within 300 km are considered further in the BART applicability modeling analysis.

TABLE 1-1. DISTANCES (KILOMETERS) SEPARATING CLASS I AREAS AND HONEYWELL'S HOPEWELL PLANT

Class I Area	Distance (km)
Breton (LA/MS)	1,340
Cape Romain (SC)	503
Chassahowitzka (FL)	1,073
Cohutta (GA)	694
Dolly Sods (WV)	**258**
Everglades (FL)	1,326
Great Smoky Mountains (NC/TN)	546
Hercules Glade (MO)	1,379
James River Face (VA)	**190**
Joyce Kilmer/Slickrock (NC)	630
Linville Gorge (NC)	437
Mammoth Cave (KY)	770
Mingo (MO)	1,137
Okefenokee (GA)	831
Otter Creek (WV)	**275**
Shenandoah (VA)	**158**
Shining Rock (NC)	537
Sipsey (AL)	963
St. Marks (FL)	1,008
Swanquarter (NC)	**227**
Wolf Island (GA)	755

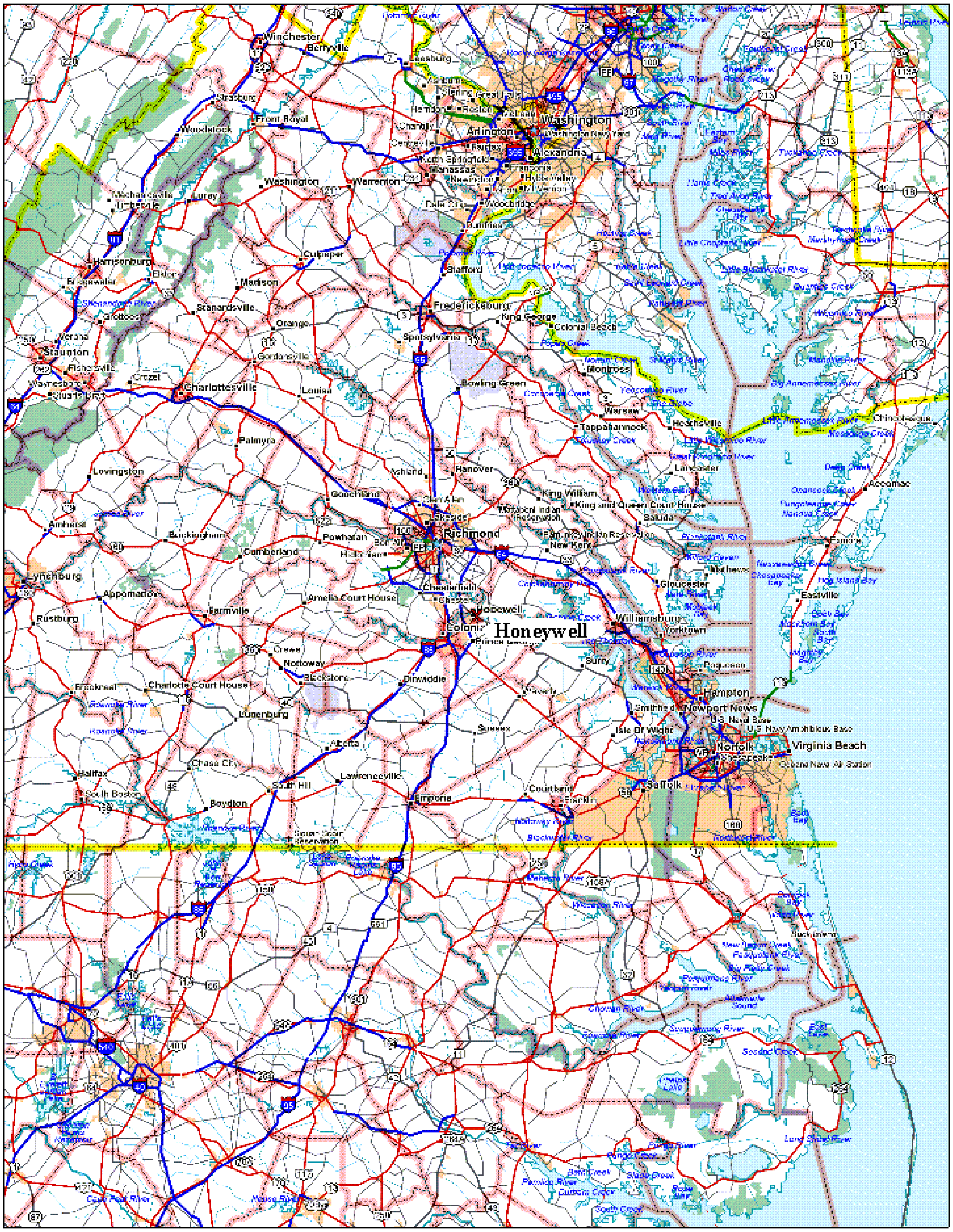
Figure 1-1 illustrates the location of the Hopewell plant, and Figure 1-2 illustrates the location of Honeywell's Hopewell plant relative to the following five federally protected Class I areas that are located within 300 km of Honeywell's Hopewell plant:

- Shenandoah National Park (NP), located approximately 158 km to the northwest of the facility, along the Blue Ridge Mountains in northwestern Virginia
- James River Face Wilderness Area (WA), located approximately 190 km to the west of the facility in central Virginia
- Swanquarter National Wildlife Refuge (NWR), located approximately 227 km to the south of the facility, along the Atlantic Coast in eastern North Carolina
- Dolly Sods Wilderness Area (WA), located approximately 258 km to the northwest of the facility in east central West Virginia
- Otter Creek Wilderness Area (WA), located approximately 275 km to the northwest of the facility in east central West Virginia

The locations of Class I areas and receptor locations evaluated in the modeling analysis were determined by, and obtained from, the U.S. Fish & Wildlife Service, the

U.S. National Park Service, and the U.S.D.A. Forest Service, which are the FLM for the Class I areas within 300 km of Honeywell's Hopewell plant.[3]

FIGURE 1-1. LOCATION OF HONEYWELL'S HOPEWELL PLANT



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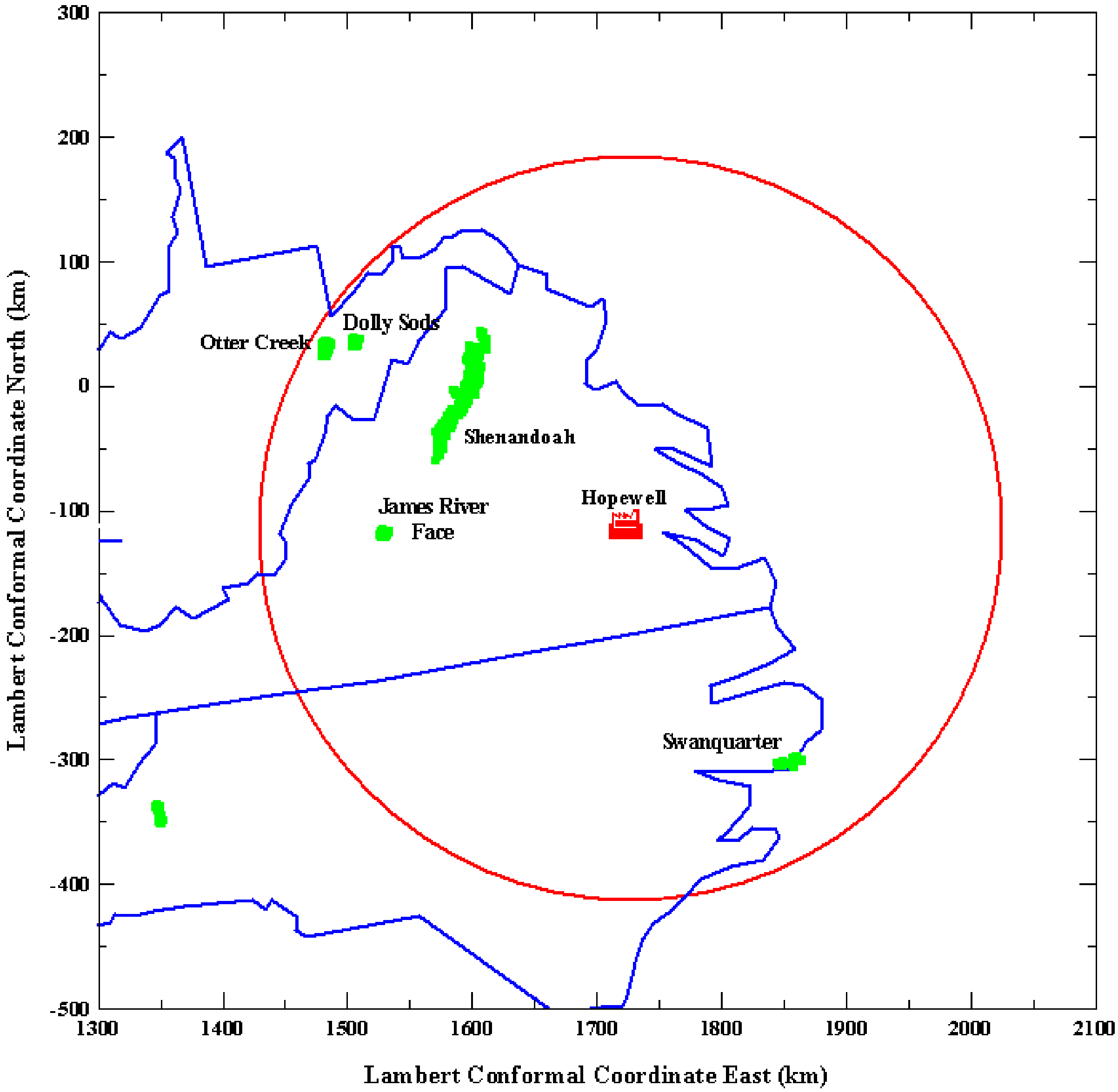
3 National Park Service compilation of Class I area receptors, http://www2.nature.nps.gov/air/maps/receptors/.

FIGURE 1-2. LOCATION OF HONEYWELL'S HOPEWELL PLANT RELATIVE TO CLASS I AREAS WITHIN 300 KM



The initial screening analysis results will be used to demonstrate whether refined analysis is necessary, and whether the scope of the refined analysis can be focused on one (or more) of the five Class I areas within 300 km. For example, should the screening analysis demonstrate that the facility does not contribute to visibility impairment at the more distant Dolly Sods, Otter Creek, and Swanquarter Class I areas, but does contribute at James River Face and Shenandoah, the refined analysis would be conducted so as to only assess visibility impairment at James River Face and Shenandoah.

Honeywell will initially conduct screening modeling of visibility impacts at all Class I areas within 300 km, but anticipates the possibility of having to conduct refined modeling of visibility impacts at one or more Class I areas, as described in this modeling protocol. Note that the *VISTAS BART Modeling Protocol* envisions the use of several refined modeling techniques (e.g., refined meteorological data sets, boundary condition emissions and CMAQ-modeled background ammonia concentrations) that are only generally described, but for which specific details were not provided. As of the date of this source-specific modeling protocol, many of these details (which are identified in this document) have still not been finalized by VISTAS. Therefore, Honeywell has identified the refined techniques that may be used in the BART applicability analysis, and anticipates additional communication with DEQ as details become available during the time between the modeling protocol submittal and applicability analysis deadline.

1.2 SCHEDULE FOR BART IMPLEMENTATION IN VIRGINIA

Each state within the VISTAS region has established its own schedule for BART implementation, which includes separate deadlines for BART applicability assessment and determination protocols and final reports. DEQ has established the following milestones for BART implementation, with which Honeywell will conform throughout the implementation process provided that DEQ and VISTAS continue to make common resources available in a timely manner.

- BART Applicability Exemption Protocol due April 15, 2006
- BART Applicability Exemption Modeling Analysis due July 5, 2006
- BART Determination Modeling Protocol due December 1, 2006
- BART Determination Modeling and Analysis, Engineering Analyses, and Permit Application due April 1, 2007

1.3 ORGANIZATION OF APPLICABILITY MODELING PROTOCOL

The remainder of this modeling protocol is organized as follows.

- Section 2 describes the BART-eligible emission units at the Hopewell plant and the emission rates to be modeled in the BART applicability analysis.
- Section 3 describes the procedural and technical guidance for conducting Class I area analyses.
- Section 4 describes the proposed approach for CALPUFF modeling, including the data resources and technical modeling options to be used in the CALMET, CALPUFF, and CALPOST analyses.
- The presentation of results from, and quality assurance techniques for, BART applicability modeling analyses are described in Section 5.

The air quality modeling analysis methodology will generally conform to the *VISTAS BART Modeling Protocol*, which is provided in Appendix A of this report for reference.

This section of the modeling protocol describes the emission units that comprise the BART-eligible source at Honeywell's Hopewell plant. Emissions and exhaust characteristics of each emission unit are quantified to demonstrate how each unit will be represented in the modeling analysis.

2.1 BART-ELIGIBLE EMISSION UNITS

Honeywell reviewed the criteria for BART-eligibility and determined that the ten emission units described in Table 2-1 comprise the BART-eligible source at the Hopewell plant.

TABLE 2-1. SUMMARY OF BART-ELIGIBLE EMISSION UNITS*

Emission Unit	Source Code/ Stack ID	BART Source Category†	Date‡ Built or Modified	Potential SO_2 Emissions (tpy)	Potential NO_X Emissions (tpy)	Potential PM_{10} Emissions (tpy)	Potential VOC Emissions (tpy)
FU-1 Kellogg Reformer	11A/103	21, 22	1960's	11	553	46	5.2
FU-6 Girdler	12A/106	21	1960's	--	81	4.9	1.0
[illegible]4 Hazardous Waste Incinerator	42A/405	21	1970's	43.8	87.1	3.2	0.35
[illegible]onium Nitrite "C" Train	90C/902	21	1965	--	[illegible]7	27.4	--
Hydroxylamine Disulfonate "C" Train	91C/907	21	1965	7.0	[illegible]5	4.5	--
Ammonium Nitrite "D" Train	90D/903	21	1966	--	600	6.0	--
Hydroxylamine Disulfonate "D" Train	91D/908	21	1966	7.0	600	4.5	--
Ammonium Nitrite "E" Train	90E/904	21	1974	--	600	6.0	--
Hydoxylamine Disulfonate "E" Train	91E/909	21	1974	8.3	600	4.5	--
Sulfuric Acid Plant	14A/108	21	1965	200	--	8.2	--
Total Potential Emissions (tpy)				**277.1**	**5,533.1**	**115.2**	**6.6**

* The emission units listed here do not include those without PM, SO_2, or NO_X emissions; the list also does not include emission units that are insignificant emission units for the Title V permitting program. Exclusion of such sources is consistent with DEQ's approach and does not change the BART eligibility demonstration since potential emissions from the listed sources exceed the exemption thresholds.

† Category 21 denotes chemical process plants; category 22 denotes large fossil fuel boilers, which for the purposes of BART eligibility include boilers individually greater than 250 MMBtu/hr that burn any amount of fossil fuel.

Honeywell's Hopewell plant is BART-eligible since potential emissions exceed 250 tpy for at least one of NO_X, SO_2, and $PM_{10,}$ which are considered visibility-affecting pollutants. Note that many of the otherwise BART-eligible emission units have potential emissions only of volatile organic compounds (VOC), which VISTAS and DEQ have determined are not visibility-affecting pollutants for the purposes of BART applicability analyses. Section 4.1.3 of the *VISTAS BART Modeling Protocol* describes the regional modeling analyses showing that cumulative VOC emissions do not contribute to visibility impairment within the VISTAS region:

> *VOC emissions from all anthropogenic point sources in each VISTAS State are being reduced. Given that the impact of eliminating all VOC emissions from all point sources in a State is less than 0.5 dv, then the impact of any one BART-eligible source would be less than 0.5 dv. Based on these analyses, the VISTAS States have concluded that VOC emissions should not be subject to BART.*

As a result of this determination, otherwise BART-eligible emission units operated by Honeywell's Hopewell plant are excluded from evaluation since these units do not emit visibility-affecting pollutants. Additionally, emission points that emit less than 5 tpy each of visibility-affecting pollutants may be excluded from the model, based on guidance from DEQ. The remaining 10 emission units are considered the BART-eligible source at Honeywell's Hopewell plant. These units include two natural gas-fired process units (reformer and girdler), a waste incinerator, a sulfuric acid plant, and three ammonium nitrite and hydroxylamine disulfonate process areas.

2.2 BART-ELIGIBLE SOURCE MODEL EMISSIONS INVENTORY

Whereas the BART eligibility determination relies on potential emissions of visibility-affecting pollutants, the BART applicability modeling analysis utilizes maximum actual 24-hour average emission rates of NO_X, SO_2, and PM_{10}. The *VISTAS BART Modeling Protocol* specifies the following hierarchy of information resources to establish the maximum actual 24-hour average emission rate for BART applicability modeling over the prior three-to-five year period:

- ▲ 24-hour maximum emissions observed using a Continuous Emission Monitor (CEM) for the period 2001 through 2003
- ▲ 24-hour maximum emissions observed using a CEM for any representative period
- ▲ Facility stack test emissions
- ▲ Potential to emit
- ▲ Permit allowable emissions
- ▲ Emissions factors from U.S. EPA *AP-42* source profiles

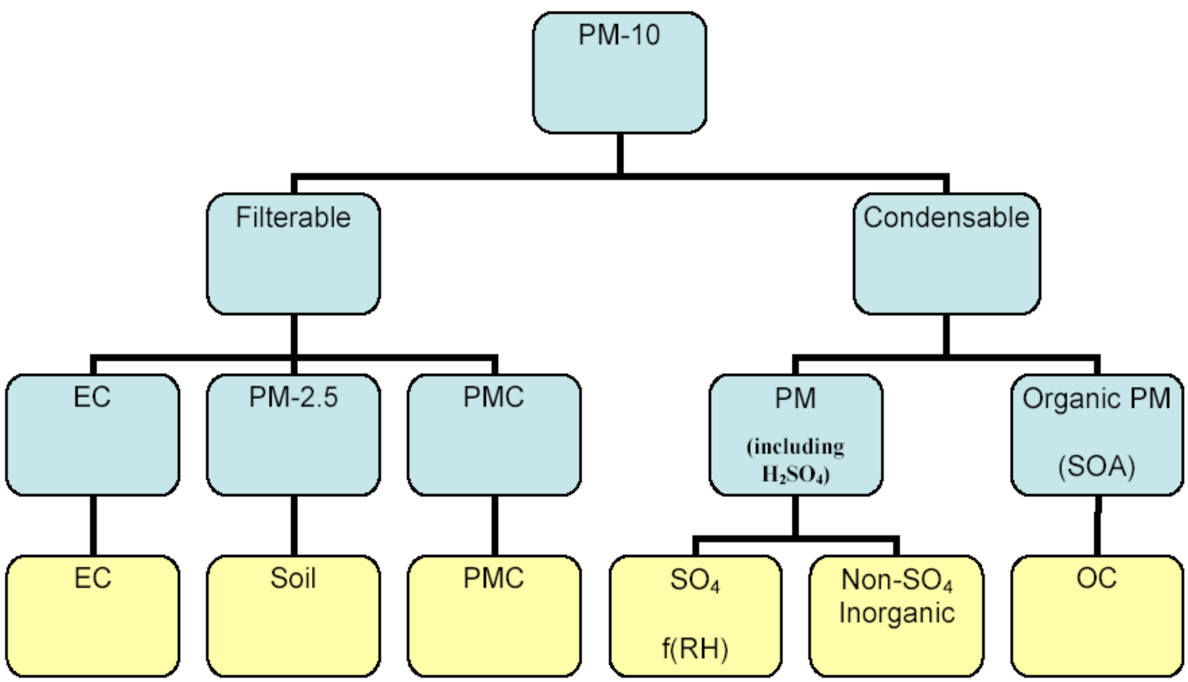
Honeywell used a combination of representative stack test data, potential emissions based on enforceable emissions and operating limits, industry-specific emission factors compiled by the EPA, and historical operating data to determine the 24-hour average maximum actual emission rates of visibility-affecting pollutants. Table 2-2 summarizes these emission rates from each BART-eligible emissions unit.

TABLE 2-2. SUMMARY OF 24-HOUR AVERAGE MAXIMUM ACTUAL EMISSION RATES

Emission Unit	NO_X Emissions (lb/hr)	SO_2 Emissions (lb/hr)	Total PM_{10} Emissions (lb/hr)	Total $PM_{2.5}$ Emissions (lb/hr)	H_2SO_4 Emissions (lb/hr)
FU-1 Kellogg Reformer	137.92	1.17	10.00	10.00	--
FU-6 Girdler	17.17	0.08	0.92	0.92	--
FU-14 Hazardous Waste Incinerator	25.00	10.00	0.88	0.78	0.15
Ammonium Nitrite "C" Train	556.66	--	6.58	6.58	--
Hydoxylamine Disulfonate "C" Train	261.00	0.17	1.08	1.08	--
Ammonium Nitrite "D" Train	183.33	--	0.16	0.16	--
Hydoxylamine Disulfonate "D" Train	235.00	0.17	0.92	0.92	--
Ammonium Nitrite "E" Train	183.33	--	0.16	0.16	--
Hydoxylamine Disulfonate "E" Train	182.50	0.42	0.83	0.83	--
Sulfuric Acid Plant	--	46.57	0.50	0.50	0.50

Table 2-2 includes 24-hour maximum emission rates of primary sulfates (as sulfuric acid mist) and distinguishes the emission rates of Total PM_{10} (TPM_{10}), which includes emissions of $TPM_{2.5}$. Modeling of visibility impairment requires that the components of the exhaust stream be speciated because different types of particulate matter affect visibility to varying extents. The amount by which a mass of a certain species scatters or absorbs light is termed the *extinction efficiency* or *extinction coefficient*, and ranges from values of 0.6 m^2/g for coarse particulate matter to 10 m^2/g for elemental carbon. Fine particulate matter (1 m^2/g) and organic aerosols (4 m^2/g) scatter light with intermediate efficiencies, and ammonium sulfate and ammonium nitrate (that forms from precursor SO_2 and NO_X emissions in the presence of ambient ammonia) are hygroscopic species that are particularly efficient light scatters in the presence of ambient water vapor ($3f(RH)$ m^2/g, where $f(RH)$ is a function of the relative humidity). The size distribution of particle species is also important, since smaller particles may be transported longer distances than larger particles and dispersed differently under prevailing ambient conditions. Figure 2-1 depicts the speciation of visibility-affecting pollutant emissions as represented in the *VISTAS BART Modeling Protocol*.

FIGURE 2-1. PARTICULATE MATTER SPECIATION
(AFTER FIGURE 4-3 OF THE *VISTAS BART MODELING PROTOCOL*)



Although the FLM have published speciation guidance for certain source types (e.g., large oil- and coal-fired combustion sources), Honeywell is not aware of specific guidance for facilities engaged in chemical manufacturing. Default speciation profiles compiled by VISTAS did not include all specific source types operated at Honeywell's Hopewell plant. Therefore, Honeywell developed the following emissions profiles based on engineering knowledge of chemical manufacturing operations and available reference data (e.g., *AP-42*).

While few data are available to estimate speciated emissions, Honeywell has reviewed what data are available to arrive at a conservative, yet reasonable estimate of speciated emissions. However, it should be noted that the data quality on PM speciation is inadequate for setting regulatory emission limits and are provided here solely as the best estimated data for a scientific analysis of potential impacts on visibility impairment at Class I areas using CALPUFF modeling. The following analysis does not represent source test results for specific sources at the Hopewell plant.

NO_X emissions from the Hopewell plant's BART-eligible sources result from combustion and processing operations. Similarly, SO_2 emissions emanate from combustion sources and processing, and result from the incomplete oxidation of fuel- or raw material-bound sulfur. Primary emissions of sulfuric acid mists or vapors, if any, are assumed to occur as only a small percentage of the primary SO_2 emissions unless an emission factor has otherwise been published. Because of the condensable nature of such emissions and the distinct effect on visibility caused by sulfates, primary sulfate is evaluated as a distinct, speciated particulate fraction. Condensable particulate matter (CPM) emissions, unlike filterable emissions, have not historically been measured or regulated for the affected sources.

PM emissions can be differentiated with respect to size, point of formation, and composition. Table 2-3 gives definitions for the nomenclature used herein.

TABLE 2-3. NOMENCLATURE FOR EMISSIONS SPECIATION ANALYSIS

Nomenclature	Description
TSP	Total suspended particulate, filterable PM with an aerodynamic diameter < 30 μm
PM_{10}	Filterable particulate matter with an aerodynamic diameter < 10 μm
PM_{6-10}	Filterable particulate matter with an aerodynamic diameter > 6 and < 10 μm
$PM_{2.5-6}$	Filterable particulate matter with an aerodynamic diameter > 2.5 and < 6 μm
$PM_{2.5}$	Filterable particulate matter with an aerodynamic diameter < 2.5 μm
$PM_{1.25-2.5}$	Filterable particulate matter with an aerodynamic diameter > 1.25 and < 2.5 μm
$PM_{1-1.25}$	Filterable particulate matter with an aerodynamic diameter > 1.0 and < 1.25 μm
$PM_{0.625-1}$	Filterable particulate matter with an aerodynamic diameter > 0.625 and < 1.0 μm
$PM_{0.5-0.625}$	Filterable particulate matter with an aerodynamic diameter > 0.5 and < 0.625 μm
CPM	Condensable particulate matter (organic and inorganic)
POC	Primary organic condensable emissions
PIC	Primary inorganic condensable emissions
TPM_{10}	Filterable PM_{10} + CPM
$TPM_{2.5}$	Filterable $PM_{2.5}$ + CPM

These PM classifications are necessary in the Class I visibility analysis because each type of PM has a different effect on visibility as defined by the extinction efficiency. The emission rates of each of these particulate phases and size categories are modeled in CALPUFF and grouped according to visibility affecting characteristics as was illustrated in Figure 2-1. Elemental carbon (EC), if emitted, typically results from unburned carbonaceous fuel and is distinguished from other PM types because of its light extinction characteristics. Coarse PM (PMC) comprises $PM_{2.5-6}$ and PM_{6-10}. Fine PM (PMF) comprises $PM_{0.5-0.625}$, $PM_{0.625-1}$, $PM_{1-1.25}$, and $PM_{1.25-2.5}$. CPM comprises both organic and inorganic species. The organic fraction of CPM is represented in CALPUFF as primary organic condensable (POC) emissions, which are direct emissions but are sometimes referred to as secondary organic aerosols (SOA) by convention and due to the representation of their visibility-affecting characteristics in the light extinction equation. Primary emissions of inorganic CPM (PIC) may contain hygroscopic sulfates (SO_4) and nitrates (NO_3), as well as other salts (e.g., carbonates) that may be hygroscopic to a lesser degree, and hence are considered in a manner similar to PMF (i.e., as soil) in terms of light extinction.[4] Therefore, it is important to distinguish inorganic CPM since certain hygroscopic species (i.e., sulfate and nitrate species) will have a greater extinction coefficient than non-hygroscopic (i.e., non-sulfate and non-nitrate) species. Even the distinction between primary sulfate and nitrate emissions is important since primary nitrate emissions will be affected by the partitioning of nitrate and nitric acid in the presence of ambient ammonia, which is modeled explicitly in CALPUFF and can be corrected when the ammonia limiting method (as described in Section 4 of this protocol) is applied. Honeywell distinguishes primary emissions of sulfates and nitrates, which would be assigned to the appropriate modeled PM type (i.e., SO4 and NO3, respectively), from non-hygroscopic species (e.g., carbonates), which would be assigned to the PIC modeled species. Inorganic condensable emissions are assumed to be PIC unless a specific emission factor for primary sulfate emissions is available.

Table 2-4 summarizes the grouping of PM species and extinction coefficient of each component. A discussion of the PM speciation methodologies for each of the BART-eligible sources at Honeywell's Hopewell plant is presented in the following sections of this protocol.

TABLE 2-4. ASSIGNMENT OF EMITTED PM SPECIES TO MODELED PM CATEGORIES

Modeled PM Category†	Components	Output Category‡	Extinction Coefficient (m^2/g)
PMC	Filterable coarse particles (PM_{6-10}, $PM_{2.5-6}$)	PMC	0.6
PMF	Filterable fine particles ($PM_{1.25-2.5}$, $PM_{1-1.25}$, $PM_{0.625-1}$, $PM_{0.5-0.625}$)	SOIL	1
PIC	Non-hygroscopic, primary inorganic condensable (PIC) emissions*	SOIL	1
SO4	Primary condensable inorganic emissions of sulfates	SO4	$3f(RH)$
NO3	Primary condensable inorganic emissions of nitrates*	NO3	$3f(RH)$
POC	Primary organic condensable emissions	SOA	4
EC	Uncombusted carbonaceous fuel	EC	10

* In the screening analyses, all condensable, non-sulfate inorganic emissions will be represented as PIC emissions. The refined analysis, if necessary, would distinguish between primary nitrate and other primary condensable inorganic emissions.

† Modeled PM Category denotes the input of emissions data into CALPUFF.

‡ Output Category denotes the assignment of modeled emissions in POSTUTIL for the visibility calculations in CALPOST.

[4] The U.S. EPA's *Guidance for Tracking Progress under the Regional Haze Rule* identifies carbonates, magnesium oxides, and sodium oxides as components of the soil mass concentration when analyzed to assess natural background visibility (Malm 1994).

2.2.1 NATURAL GAS COMBUSTION UNITS PARTICULATE SPECIATION

Honeywell operates the natural gas-fired Kellogg reformer (Permit Emission Unit 11A) and Girdler Unit (Permit Emission Unit 12A). Particulate emissions occur through combustion of natural gas, which is a raw material in the process. To speciate the PM emissions from these gas-fired combustion sources, Honeywell utilized PM size fractions and CPM emissions information from Section 1.4 of U.S. EPA's *AP-42* emission factor database.[5] Honeywell also referred to the National Park Service (NPS) guidance for speciation of natural gas combustion sources, which notes that all fine particulate matter should be considered elemental carbon.[6] Finally, a recent study for the National Petroleum Technology Office of the U.S. Department of Energy was utilized to determine the organic and inorganic portions of CPM.[7] Table 2-5 summarizes the relevant data for this category of sources.

TABLE 2-5. KELLOGG REFORMER/GIRDLER SPECIATION DATA

Speciation Data	Value	Reference
Organic portion of CPM	89.9%	U.S. DOE Study, Table 3-11
Inorganic portion of CPM	10.2%	
Filterable portion of TPM_{10}	25.0%	
Condensable portion of TPM_{10}	75.0%	
PM_{6-10} as a % of PM_{10}*	0.0%	
$PM_{2.5-6}$ as a % of PM_{10}*	0.0%	
$PM_{1.25-2.5}$ as a % of PM_{10}*	0.0%	
$PM_{1-1.25}$ as a % of PM_{10}*	0.0%	
$PM_{0.625-1}$ as a % of PM_{10}†	15.0%	
$PM_{0.5-0.625}$ as a % of PM_{10}†	85.0%	

* AP-42 states that all PM (total, condensable, and filterable) is assumed to be less than 1.0 micrometer in diameter.

† AP-42 does not provide size speciation. However, the U.S. DOE study for site Delta indicates that 7% of filterable PM is greater than 0.625 microns and an additional 16% is between 0.32 and 1.0 microns. 7% plus 8% (half of the 16% attributed to the 0.32 to 1.0 size category in the study) is considered to be $PM_{0.625-1.0}$ for BART speciation purposes. The remaining filterable PM was attributed $PM_{0.5-0.625}$.

As noted previously, NPS guidance suggests fine filterable PM emissions are to be modeled as elemental carbon. The *AP-42* emission factors for natural gas combustion indicate that all PM emissions from natural gas combustion are less than 1 micrometer; therefore, there are no coarse PM (PMC) emissions from these natural gas-fired units. Similarly, there are no fine, filterable PM emissions (PMF) modeled, since all filterable emissions are allocated to elemental carbon. Condensable emissions are allocated between

[5] AP-42, Section 1.4, *Natural Gas Combustion,* Table 1.4-2*,* July 1998.

[6] http://www2.nature.nps.gov/air/permits/emissions_ControlTech.cfm

[7] England, Glenn. *Development of Fine Particulate Emission Factors and Speciation Profiles for Oil- and Gas-Fired Combustion Systems.* October 2004. http://www.nyserda.org/programs/Environment/EMEP/project/6230/6230_pwp.asp

primary organic (POC) and inorganic species (PIC), which includes sulfates and nitrates. Pipeline quality natural gas combustion results in little sulfur emissions due to negligible fuel sulfur content. However, Honeywell has represented maximum actual emissions as potential sulfur dioxide emissions for the purposes of BART applicability modeling, while sulfuric acid emissions are assumed to be negligible.

TPM_{10} and $TPM_{2.5}$ emissions, which are equivalent for natural gas combustion sources, are 10.0 lb/hr for the reformer and 0.92 lb/hr for the girdler.

Organic CPM emissions were determined by multiplying the calculated TPM_{10} emissions by the condensable percentage of TPM_{10} and the organic percentage of CPM. Organic CPM was assumed to be evenly split between the two size categories, 0.625-1.0 μm and 0.5-0.625 μm. The organic CPM calculation for the reformer is shown below.

$$\left(10.0\frac{\text{lb TPM}_{10}}{\text{hr}}\right)\left(75\%\frac{\text{CPM}}{\text{TPM}_{10}}\right)\left(89.9\%\frac{\text{organic CPM}}{\text{CPM}}\right)/2 = 3.37\frac{\text{lb organic CPM for each size category}}{\text{hour}}$$

Non-sulfate inorganic CPM emissions were calculated based on subtracting the organic CPM emissions and the H_2SO_4 emissions (assumed to be negligible) from the total CPM emissions. The non-sulfate inorganic CPM emissions were split evenly between the two size categories, 0.625-1.0 μm and 0.5-0.625 μm.

Filterable PM_{10} emissions were divided amongst six different size categories by multiplying TPM_{10} emissions by the filterable % and then by the % of PM_{10} for each size category, yielding hourly emissions of $PM_{6\text{-}10}$, $PM_{2.5\text{-}6}$, $PM_{1.25\text{-}2.5}$, $PM_{1\text{-}1.25}$, $PM_{0.625\text{-}1}$, and $PM_{0.5\text{-}0.625}$. A sample calculation for $PM_{0.5\text{-}0.625}$ from the reformer is shown below. Note that all filterable PM less than 2.5 microns in size was assumed to be elemental carbon.

$$\left(10.0\frac{\text{lb TPM}_{10}}{\text{hr}}\right)\left(25\%\frac{\text{PM}_{10}}{\text{TPM}_{10}}\right)\left(85\%\frac{\text{PM}_{0.5\text{-}0.625}}{\text{PM}_{10}}\right) = 2.13\frac{\text{lb PM}_{0.5\text{-}0.625}}{\text{hour}}$$

Table 2-6 presents a summary of the speciated PM emissions for the reformer and girdler. Figures 2-2 and 2-3, respectively, presents graphical representations for the total 10.0 lb/hr of TPM_{10} from the reformer and 0.92 lb/hr of TPM_{10} from the girdler

TABLE 2-6. KELLOGG REFORMER/GIRDLER PM SPECIATED EMISSIONS (LB/HR)

Unit	POC (µm)		PIC (non-sulfate) (µm)		SO_4	PMC (µm)	PMF (µm)	EC (µm)	
	0.625-1.0	0.5-0.625	0.625-1.0	0.5-0.625		2.5-10	0.5-2.5	0.625-1.0	0.5-0.625
Reformer	3.37	3.37	0.38	0.38	--	--	--	0.38	2.13
Girdler	0.31	0.31	0.035	0.035	--	--	--	0.035	0.20

FIGURE 2-2. KELLOGG REFORMER TPM_{10} SPECIATION (LB/HR)

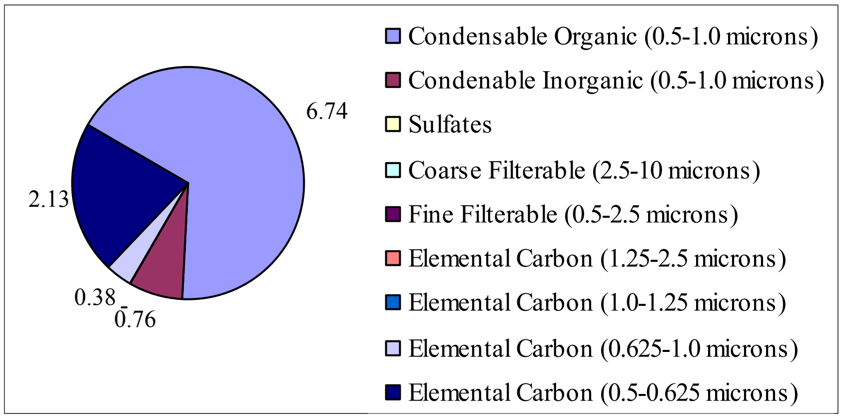
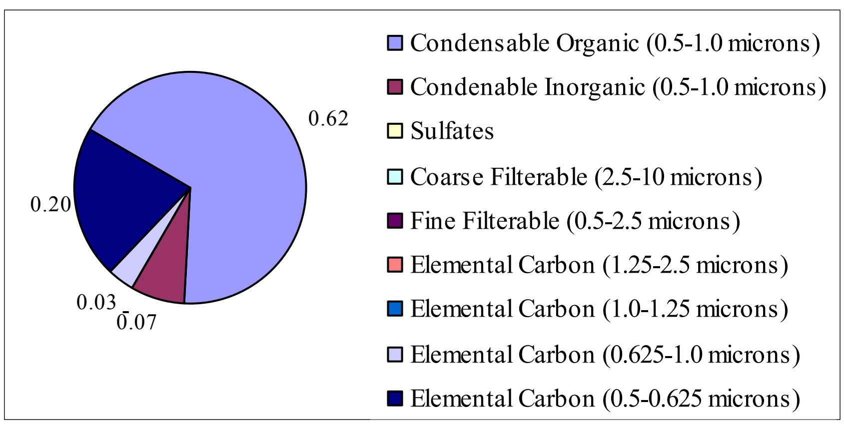


FIGURE 2-3. GIRDLER TPM_{10} SPECIATION (LB/HR)



2.2.2 WASTE INCINERATOR PARTICULATE SPECIATION

Honeywell operates the distillate-fired waste incinerator (Permit Emission Unit 42A) without an add-on PM control device. The waste incinerator is authorized to combust waste from the Specialty Chemicals area. Particulate emissions occur through combustion of this waste. To speciate the PM emissions from this source, Honeywell utilized PM size fractions and CPM emissions information from Section 1.3 of U.S. EPA's *AP-42* emission factor database.[8] Honeywell also referred to the National Park Service (NPS) guidance for speciation of oil-fired combustion sources, which notes that half of all filterable particulate matter should be considered elemental carbon and half should be considered soils.[9] Table 2-7 summarizes the relevant data for this category of sources.

TABLE 2-7. WASTE INCINERATOR SPECIATION DATA

Speciation Data	Value	Reference
EC as a % of Fine PM_{10}	50.0%	NPS Guidance for Fuel Oil Combustion
Organic portion of CPM	35.0%	AP-42 Section 1.3, Tables 1.3.1, 1.3.2, 1.3.7 Fuel Oil Combustion, Distillate-Fired Boilers*
Inorganic portion of CPM	65.0%	
TPM_{10} as a % of TSP	120.0%	
Filterable portion of TPM_{10}	45.8%	
Condensable portion of TPM_{10}	54.2%	
PM_{6-10} as a % of PM_{10}	10.9%	
$PM_{2.5-6}$ as a % of PM_{10}	12.7%	
$PM_{1.25-2.5}$ as a % of PM_{10}	7.3%	
$PM_{1-1.25}$ as a % of PM_{10}	1.8%	
$PM_{0.625-1}$ as a % of PM_{10}	3.6%	
$PM_{0.5-0.625}$ as a % of PM_{10}	63.6%	

* Size values provided in AP-42 were expressed as a % of TSP and were converted to % as PM_{10} by dividing by the % of TSP that is PM_{10} (as shown in the AP-42 table). For example, PM_{6-10} is calculated as $(PM_{10}\% - PM_6\%)/(PM_{10}\%) = PM_{6-10}$ as % of PM_{10}.

Using the information presented in Table 2-7, Honeywell first calculated TPM_{10} emissions by multiplying the maximum hourly TSP emission rate of 0.73 lb/hr by 120.0%, yielding 0.88 lb/hr TPM_{10}. $TPM_{2.5}$ emissions were calculated based on TPM_{10} emissions minus coarse filterable PM_{10} emissions (PM_{6-10} and $PM_{2.5-6}$).

Next, the organic CPM emissions were determined by multiplying the calculated TPM_{10} emissions by the condensable % of TPM_{10} and the organic % of CPM. Organic CPM was assumed to be evenly split between the two size categories, 0.625-1.0 μm and 0.5-0.625 μm. The organic CPM calculation is shown below.

$$\left(0.88\,\frac{\text{lb TPM}_{10}}{\text{hr}}\right)\left(54.2\%\,\frac{\text{CPM}}{\text{TPM}_{10}}\right)\left(35.0\%\,\frac{\text{organic CPM}}{\text{CPM}}\right)/\,2 = 0.083\,\frac{\text{lb organic CPM for each size category}}{\text{hour}}$$

Non-sulfate inorganic CPM emissions were calculated based on subtracting the organic CPM emissions and the H_2SO_4 emissions from the total CPM emissions (which were based on 1% conversion of fuel sulfur to sulfate). The non-sulfate inorganic CPM emissions were split evenly between the two size categories, 0.625-1.0 μm and 0.5-0.625 μm.

[8] AP-42, Section 1.3, *Fuel Oil Combustion,* Tables 1.3-1, 1.3-2, 1.3-7*,* September 1998.

[9] http://www2.nature.nps.gov/air/permits/emissions_ControlTech.cfm

Filterable PM_{10} emissions were divided amongst six different size categories by multiplying TPM_{10} emissions by the filterable percentage and then by the percentage of PM_{10} for each size category, yielding hourly emissions of PM_{6-10}, $PM_{2.5-6}$, $PM_{1.25-2.5}$, $PM_{1-1.25}$, $PM_{0.625-1}$, and $PM_{0.5-0.625}$. For fine particulate emissions, PM less than 2.5 microns, the calculated emissions must also be multiplied by the portion of fine particulate that is not EC, i.e., 100% - 50%, since EC is included in the percentages of filterable PM shown in Table 2-7 for $PM_{1.25-2.5}$, $PM_{1-1.25}$, $PM_{0.625-1}$, and $PM_{0.5-0.625}$.

Sample calculations for PM_{6-10} and $PM_{1.25-2.5}$ are shown below.

$$\left(0.88\,\frac{\text{lb TPM}_{10}}{\text{hr}}\right)\left(45.8\%\,\frac{\text{PM}_{10}}{\text{TPM}_{10}}\right)\left(10.9\%\,\frac{\text{PM}_{6\text{-}10}}{\text{PM}_{10}}\right) = 0.44\,\frac{\text{lb PM}_{6\text{-}10}}{\text{hour}}$$

$$\left(0.88\,\frac{\text{lb TPM}_{10}}{\text{hr}}\right)\left(45.8\%\,\frac{\text{PM}_{10}}{\text{TPM}_{10}}\right)\left(7.3\%\,\frac{\text{PM}_{1.25\text{-}2.5}}{\text{PM}_{10}}\right)\left(100\% - 50\%\,\frac{\text{EC}}{\text{PM}_{10}}\right) = 0.015\,\frac{\text{lb PM}_{1.25\text{-}2.5}}{\text{hour}}$$

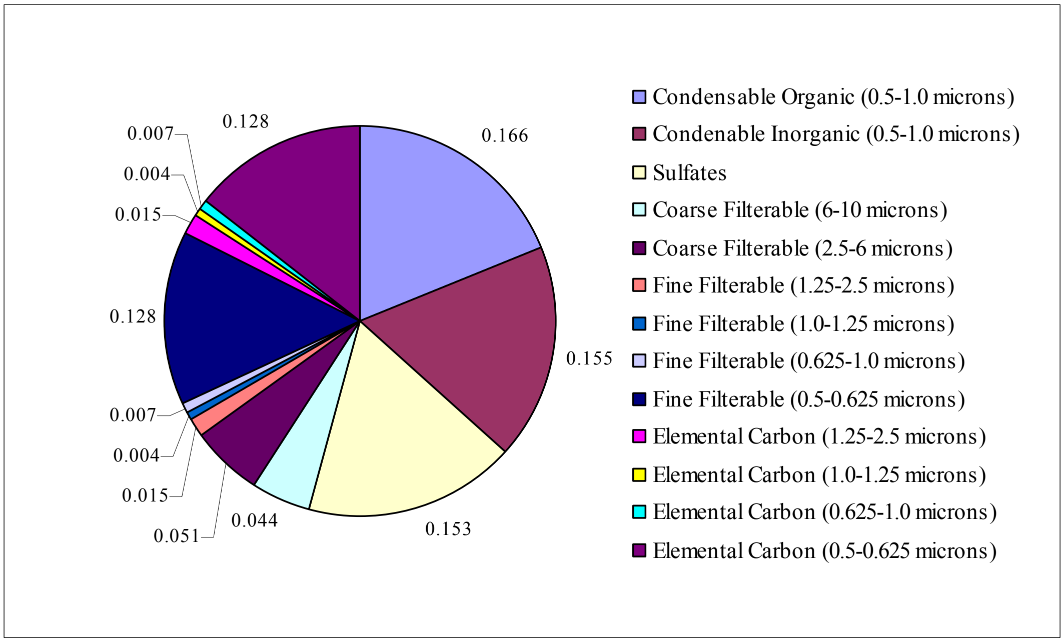
All EC was presumed to be divided amongst the size categories based on the AP-42 percentages.

Table 2-8 presents a summary of the speciated PM emissions for the waste incinerator. Figure 2-4 presents graphical representations of the speciated TPM_{10} emissions of 0.88 lb/hr for the waste incinerator.

TABLE 2-8. WASTE INCINERATOR PM SPECIATED EMISSIONS (LB/HR)

POC (µm)		PIC (non-sulfate) (µm)			PMC (µm)		PMF (µm)				EC
0.625-1.0	**0.5-0.625**	**0.625-1.0**	**0.5-0.625**	**SO_4**	**6-10**	**2.5-6**	**1.25-2.5**	**1.0-1.25**	**0.625-1.0**	**0.5-0.625**	**0.5-0.625**
0.083	0.083	0.078	0.078	0.15	0.044	0.051	0.015	0.0037	0.0073	0.13	0.15

FIGURE 2-4. WASTE INCINERATOR TPM_{10} SPECIATION (LB/HR)



2.2.3 AMMONIUM NITRITE TRAINS PARTICULATE SPECIATION

Honeywell operates three BART-eligible ammonium nitrite trains (Permit Emission Units 90C, 90D, and 90E) equipped with wet scrubbers. The wet scrubbers are operated at a low (50-60°F) temperature and the particulate emissions are anticipated to be primarily ammonium nitrite, which is readily soluble in the water in the scrubbers. Therefore, condensable particulate matter is anticipated to be removed in the wet scrubber and any remaining particulate emissions from these units are assumed to be filterable. Furthermore, the raw material feed to the ammonium nitrite trains contains carbonaceous material derived from natural gas. Therefore, Honeywell has conservatively assumed that the filterable particulate matter emissions are elemental carbon and used the speciation information for natural gas combustion discussed in Section 2.2.1. Table 2-9 summarizes the relevant speciation data for this source.

TABLE 2-9. AMMONIUM NITRITE TRAIN PM SPECIATED EMISSIONS (LB/HR)

	POC (µm)		PIC (non-sulfate) (µm)			PMC (µm)	PMF (µm)	EC (µm)	
Train	0.625-1.0	0.5-0.625	0.625-1.0	0.5-0.625	SO_4	2.5-10	0.5-2.5	0.625-1.0	0.5-0.625
C	--	--	--	--	--	--	--	0.99	5.60
D	--	--	--	--	--	--	--	0.024	0.13
E	--	--	--	--	--	--	--	0.024	0.13

2.2.4 HYDROXYLAMINE DISULFONATE TRAINS PARTICULATE SPECIATION

Honeywell operates three BART-eligible hydroxylamine disulfonate trains (Permit Emission Units 91C, 91D, and 91E) equipped with wet scrubbers. The wet scrubbers are operated at a low (50-60°F) temperature and the particulate emissions are anticipated to be primarily sulfonates, which is readily soluble in the water in the scrubbers. Therefore, condensable particulate matter is anticipated to be removed in the wet scrubber and particulate emissions from these units are assumed to be filterable. Furthermore, the raw material feed to the hydroxylamine disulfonate trains contains carbonaceous material derived from natural gas. Therefore, Honeywell has conservatively assumed that the filterable particulate matter emissions are elemental carbon and used the speciation information for natural gas combustion discussed in Section 2.2.1. Table 2-10 summarizes the relevant speciation data for this source.

TABLE 2-10. HYDROXYLAMINE DISULFONATE TRAIN PM SPECIATED EMISSIONS (LB/HR)

Train	POC (μm) 0.625-1.0	POC (μm) 0.5-0.625	PIC (non-sulfate) (μm) 0.625-1.0	PIC (non-sulfate) (μm) 0.5-0.625	SO_4	PMC (μm) 2.5-10	PMF (μm) 0.5-2.5	EC (μm) 0.625-1.0	EC (μm) 0.5-0.625
C	--	--	--	--	--	--	--	0.16	0.92
D	--	--	--	--	--	--	--	0.14	0.78
E	--	--	--	--	--	--	--	0.12	0.71

2.2.5 SULFURIC ACID PLANT PARTICULATE SPECIATION

Honeywell operates a sulfuric acid plant (Permit Emission Unit 14A) with no add-on control device for PM. The TPM_{10} emissions of 0.5 lb/hr were assumed to be all in the form of sulfuric acid mist.

2.3 MODELED STACK PARAMETERS AND EMISSIONS

Actual stack parameters will be input to the CALPUFF model to represent the point of visibility-affecting pollutant emissions. The location of each point source will be represented consistently in the Lambert Conformal Coordinate system used for the screening and refined meteorological data analyses prepared by VISTAS. Each exhaust discharges vertically without obstruction. Since the nearest Class I area is located more than 150 km to the facility, effects of building downwash will not be considered unless specifically requested by DEQ. Table 2-11 summarizes the stack parameters and Table 2-12 summarizes the modeled emission rates for BART-eligible emission units at Honeywell's Hopewell plant.

TABLE 2-11. STACK PARAMETERS FOR BART-ELIGIBLE EMISSION UNITS

Emission Unit	Stack ID	UTM East (km)	UTM North (km)	Stack Height (feet)	Stack Diameter (feet)	Exhaust Temperature (°F)	Exhaust Velocity (feet/sec)
FU-1 Kellogg Reformer	103	298.6	4,130.6	105	11.30	238	44.89
FU-6 Girdler	106	298.6	4,130.6	50	5.00	320	21.66
FU-14 Hazardous Waste Incinerator	405	298.6	4,130.6	150	2.50	185	40.74
Ammonium Nitrite “C” Train	902	298.6	4,130.6	125	1.33	41	114.09
Hydoxylamine Disulfonate “C” Train	907	298.6	4,130.6	132	2.00	59	59.95
Ammonium Nitrite “D” Train	903	298.6	4,130.6	125	1.33	41	114.09
Hydoxylamine Disulfonate “D” Train	908	298.6	4,130.6	132	2.00	63	59.95
Ammonium Nitrite “E” Train	904	298.6	4,130.6	115	2.00	41	65.25
Hydoxylamine Disulfonate “E” Train	909	298.6	4,130.6	112	2.00	63	76.96
Sulfuric Acid Plant	108	298.6	4,130.6	185	5.00	100	55.20

TABLE 2-12. MODELED EMISSION RATES FOR BART-ELIGIBLE EMISSION UNITS

Emission Unit	Stack ID	POC (lb/hr)		PIC (lb/hr)		PMC (lb/hr)		PMF (lb/hr)				EC (lb/hr)				Sulfate (lb/hr)
		6-10 µm	2.5-6 µm	0.625-1.0 µm	0.5-0.625 µm	6-10 µm	2.5-6 µm	1.25-2.5 µm	1.0-1.25 µm	0.625-1.0 µm	0.5-0.625 µm	1.25-2.5 µm	1.0-1.25 µm	0.625-1.0 µm	0.5-0.625 µm	
FU-1 Kellogg Reformer	103	3.37	3.37	0.38	0.38	--	--	--	--	--	--	--	--	0.38	2.13	--
FU-6 Girdler	106	0.31	0.31	0.035	0.035	--	--	--	--	--	--	--	--	0.035	0.20	--
FU-14 Hazardous Waste Incinerator	405	0.083	0.083	0.078	0.078	0.044	0.051	0.015	0.0037	0.0073	0.13	0.015	0.0037	0.0073	0.13	0.15
Ammonium Nitrite “C” Train	902	--	--	--	--	--	--	--	--	--	--	--	--	0.99	5.60	--
Hydoxylamine Disulfonate “C” Train	907	--	--	--	--	--	--	--	--	--	--	--	--	0.16	0.92	--
Ammonium Nitrite “D” Train	903	--	--	--	--	--	--	--	--	--	--	--	--	0.024	0.13	--
Hydoxylamine Disulfonate “D” Train	908	--	--	--	--	--	--	--	--	--	--	--	--	0.14	0.78	--
Ammonium Nitrite “E” Train	904	--	--	--	--	--	--	--	--	--	--	--	--	0.024	0.13	--
Hydoxylamine Disulfonate “E” Train	909	--	--	--	--	--	--	--	--	--	--	--	--	0.12	0.71	--
Sulfuric Acid Plant	108	--	--	--	--	--	--	--	--	--	--	--	--	--	--	0.50

3. GEOPHYSICAL AND METEOROLOGICAL DATA

Section 3 of this BART applicability modeling protocol for Honeywell's Hopewell plant describes the geophysical and meteorological data that will be used in the screening and refined analyses. The information in this Section 3 is largely adapted from the *VISTAS BART Modeling Protocol*, which is presented in Appendix A of this source-specific protocol for reference, and sample model files made available on the VISTAS technical contractor website.[10]

CALMET requires geophysical data about the domain to characterize the terrain and land use parameters that potentially affect dispersion. Terrain features affect flows and create turbulence in the atmosphere and are potentially subjected to higher concentrations of elevated puffs, and different land uses exhibit variable characteristics such as surface roughness, albedo, Bowen ratio, and leaf-area index that also affect turbulence and dispersion.

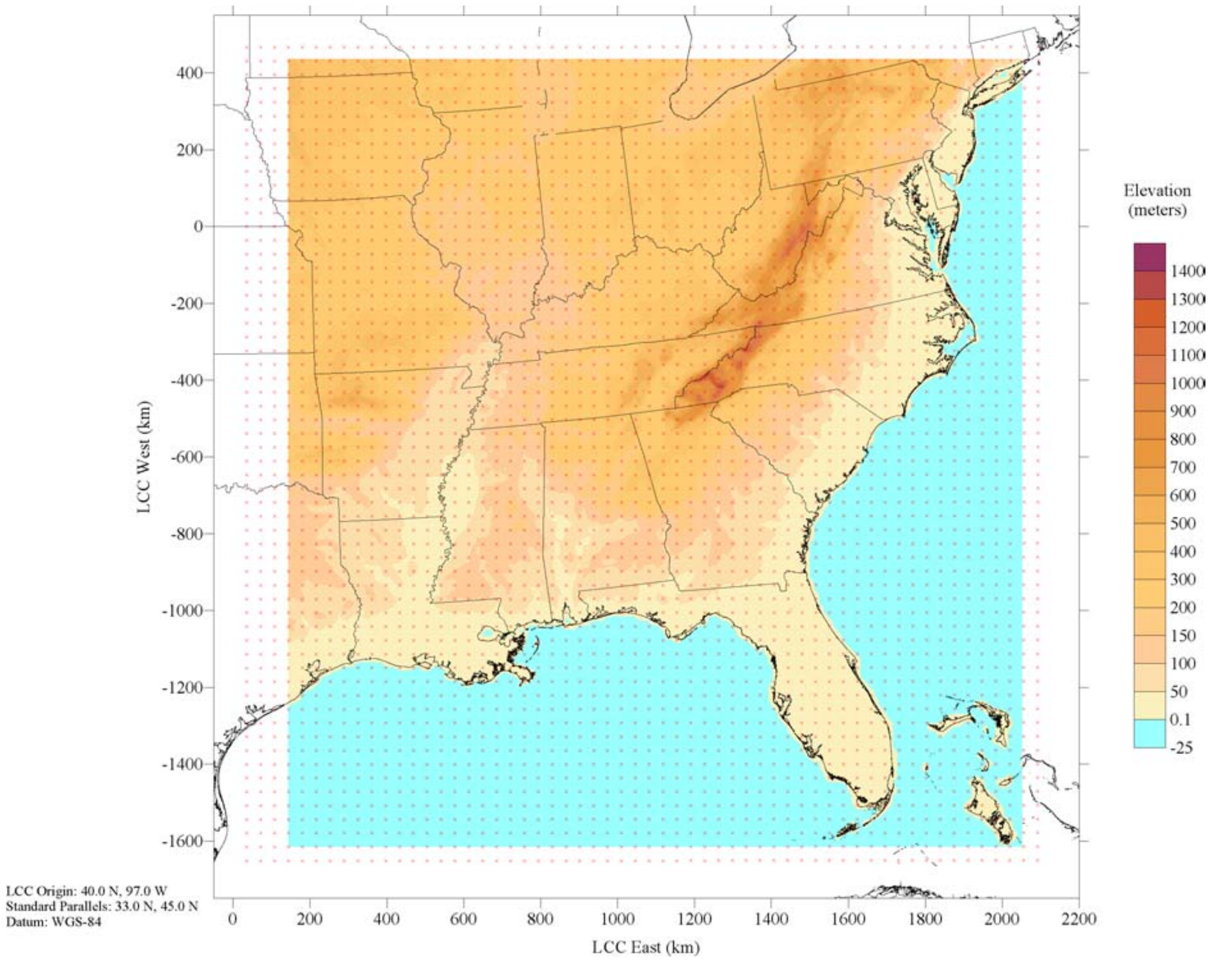
3.1 TERRAIN ELEVATIONS WITHIN THE MODELING DOMAIN

Terrain elevations within the modeling domain were processed from SRTM-GTOPO30 digital terrain data format with 30-arcsec resolution. SRTM30 is a digital elevation data set that spans the globe from 60° north latitude to 56° south latitude, approximately from the southern tip of Greenland to below the southern tip of South America. It has a horizontal grid spacing of 30 arc-seconds (approximately 1 kilometer). GTOPO30 is a global digital elevation model with a horizontal grid spacing of 30 arc-seconds (approximately 1 kilometer) that was derived from several raster and vector sources of topographic information that include U.S. Geological Survey digital elevation models. The VISTAS technical contractor used data preprocessors to format and assimilate these data into a single geophysical data file for processing by CALMET. The representation of terrain in the regional screening analysis resolves the terrain onto the 12-km regional grid used for screening modeling depicted in Figure 3-1.

Refined analyses may be necessary as part of the Honeywell BART applicability analysis, in which case CALMET grid sizes of 4 km or less (e.g., 1 km) would be used to represent the modeling domain. As described in the *VISTAS BART Modeling Protocol*, VISTAS intends to provide 2001 through 2003 CALMET files for five 4-km sub-regional domains, one of which appears to include Honeywell's Hopewell plant and the five Class I areas within 300 km. The *VISTAS BART Modeling Protocol* envisions the use of higher resolution terrain DEM data (e.g., 3 arc-second U.S. Geological Survey data) for this analysis.

[10] http://src.com/verio/download/download.htm#VISTAS_VERSION.

FIGURE 3-1. TERRAIN REPRESENTATION IN THE 12-KM REGIONAL SCREENING GRID (AFTER FIGURE 4-2 OF THE *VISTAS BART MODELING PROTOCOL*)



3.2 LAND USE AND COVER WITHIN THE MODELING DOMAIN

Land use and land cover (LULC) within the modeling domain was assimilated by the VISTAS technical contractor into a single geophysical data file for processing by CALMET using Composite Theme Grid (CTG) data archived by the U.S. Geological Survey at a resolution of 200 meters. CALMET was used to calculate the fractional land use types within each cell of the 12-km size regional grid. LULC in each grid cell was used by CALMET to compute the micrometeorological parameters (i.e., surface roughness, Bowen ratio, albedo, soil heat flux) that affect turbulent dispersion in the boundary layer.

Refined analyses may be necessary as part of the Honeywell BART applicability analysis, in which case CALMET grid resolutions of 4 km or less (e.g., 1 km) would be used to represent the modeling domain. As described in the *VISTAS BART Modeling Protocol*, VISTAS intends to provide 2001 through 2003 CALMET files for five 4-km sub-regional domains, one of which appears to include Honeywell's Hopewell plant and the five Class I areas. The *VISTAS BART Modeling Protocol* does not explicitly indicate that higher resolution LULC data would be used for a refined analysis; therefore the 200-meter CTG format will provide adequate resolution for CALMET grid spacing down to 1 km. Therefore, refined analyses performed by Honeywell, if necessary, will utilize the same CTG LULC data.

3.3 METEOROLOGICAL DATABASE

CALMET is the meteorological preprocessor that compiles three-dimensional meteorological fields from mesoscale model (MM) output, raw observations of surface and upper air conditions, precipitation measurements, and geophysical parameters into a single hourly, gridded data set for input to CALPUFF. The federal *Guideline* for CALPUFF processing provides the following recommendations for the meteorological data period at Section 9.3.1.2:

> *Less than five, but at least three, years of meteorological data (need not be consecutive) may be used if mesoscale meteorological fields are available, as discussed in paragraph 9.3(c). These mesoscale meteorological fields should be used in conjunction with available standard [National Weather Service] NWS or comparable meteorological observations within and near the modeling domain.*

The *VISTAS BART Modeling Protocol* describes a regional domain and a set of pre-computed regional CALMET meteorological files with 12 km grid size for the years 2001, 2002, and 2003, prepared by the VISTAS technical contractor to allow any Class I areas within the VISTAS area to be evaluated with a consistent meteorological database and consistent CALPUFF modeling options. The CALMET modeling output files in the form of CALPUFF-ready three-dimensional meteorological files were made available on external hard drives to the States and other parties. These data were obtained by Honeywell's technical contractor and will be utilized in the regional screening analyses. Should refined analyses be necessary, Honeywell will initially utilize one of the 4-km refined CALMET grids provided by VISTAS, also for the 2001 through 2003 data period. Higher resolution analyses, should they be conducted (for example with 1 km grid spacing), would also be prepared for this data period using the resources described in the following sections.

3.3.1 MM5 SIMULATIONS

MM data are used as "observed" or "first-guess" fields in CALMET due to its high-resolution representation of meteorological conditions on a uniform three-dimensional grid. The following three years of MM5 meteorological data have been assembled by VISTAS for use in the regional CALPUFF modeling effort:

- 2001 MM5 dataset at 12 km and 36 km grid (developed for EPA)
- 2002 MM5 dataset at 12 km and 36 km grid (developed by VISTAS)
- 2003 MM5 dataset at 36 km grid (developed by the Midwest Regional Planning Organization).

These data sets were provided to the VISTAS technical contractor, which produced annual CALMET meteorological files at for the 12-km grid resolution regional domain. The development of the regional CALMET meteorological fields from MM5 data were conducted in No-Observations ("No-Obs") mode since the MM5 data already reflect assimilation of observational data and are likely to adequately characterize regional wind patterns that are consistent with the 12-km grid scale.

When the 12-km MM5 (2001 and 2002) data are used, the diagnostic CALMET terrain adjustments were turned off since the grid resolution of the MM5 data is the same as the CALMET grid and the terrain adjustments on the 12-km grid scale will already be reflected in the MM5 dataset. In this case, the MM5 winds will be interpolated by CALMET to the CALMET layers and CALMET's boundary layer modules will compute mixing heights, turbulence parameters and other meteorological parameters that are required by CALPUFF. For 2003, the 36-km MM5 data were used as CALMET's initial guess field and then the CALMET diagnostic terrain adjustments (see Section 3.1.1 of the *VISTAS BART Modeling Protocol*) were applied to reflect terrain on the scale of the CALMET grid (i.e., 12 km).

3.3.2 MEASUREMENTS AND OBSERVATIONS

The finer grid (4 km) CALMET simulations, which Honeywell may utilize should a refined analysis be necessary, will be run by VISTAS technical contractor in hybrid mode, using both MM5 data to define the initial guess fields and NWS meteorological observational data in the Step 2 calculations. In this manner, actual observations of three-dimensional meteorological conditions can be used in the model to smooth the coarse MM5 resolution to better represent areas in which terrain features and coastlines may have an important effect on meteorological conditions, but not be well resolved in the mesoscale model. Surface, upper air, precipitation, and offshore buoy observation points are readily available for use in CALMET. As of the date of this modeling protocol, the VISTAS technical contractor has not completed the refined CALMET analyses; hence the specific observations used have not been identified. The following generally describes the use of NWS observations in Step 2 of the CALMET analyses.

Parameters affecting turbulent dispersion that are observed hourly at surface stations include wind speed and direction, temperature, cloud cover and ceiling, relative humidity, and precipitation type. Surface data would be selected from the available data inventory to optimize spatial coverage and representation of the domain. Raw observations would be obtained from the National Climatic Data Center (NCDC), quality assured, and merged using the SMERGE pre-processor to create a single assimilated data file of surface observations for each year analyzed.

Observations of meteorological conditions in the upper atmosphere provide a profile of turbulence from the surface through the depth of the boundary layer in which dispersion occurs. Upper air data are collected by balloons launched simultaneously across the observation network at 0000 Greenwich Mean Time (GMT) (5 o'clock PM in Virginia) and 1200 GMT (5 o'clock AM in Virginia). Sensors observe pressure, wind speed and direction, and temperature (among other parameters) as the balloon rises through the atmosphere. The upper air observation network is less dense than surface observation points since upper air conditions vary less and are generally not as affected by local effects (e.g., terrain or coastlines). Upper air data would be extracted from the NCDC's available data inventory to optimize spatial coverage and representation of the domain, and utilization from year to year may vary due to availability and data quality.

The effects of wet deposition processes on ambient pollutant concentrations are an important part of the BART applicability analysis. Therefore, it is necessary to include observations of precipitation in the CALMET analysis. Precipitation data would be collected from selected surface meteorological data stations included in the analysis, plus Cooperative Observation Network (COOP) stations nearer to or within the domain. Precipitation data were extracted from among the NCDC's available data inventory to optimize spatial coverage and representation of the domain. Raw observations from these stations would be quality assured and merged using the PMERGE pre-processor to create a single assimilated data file of precipitation observations.

Because parts of the modeling domain encompass the open waters of the Atlantic Ocean and the Swanquarter Class I area is located along the Atlantic Coast, meteorological data from coastal and offshore buoys can be useful so that overwater meteorological processing algorithms in CALMET can be utilized. The critical differences in behavior of the inland and marine boundary layers, and atmospheric dispersion phenomena occurring within these distinct regimes, is well documented and recognized to play a vital role in the dispersion of pollutants originating in, or destined to affect, coastal areas. Key phenomena occurring in coastal environments that affect pollutant dispersion include land/sea-breezes that cause recirculation of pollutant mass, temperature moderation that results in sharp gradients and mixing height discontinuities at the land-sea interface, and thermal internal boundary layers that could cause severe fumigation under certain conditions. The CALMET processor is equipped to assimilate overwater data obtained from coastal, near-shore, and offshore observation platforms. CALMET uses a profile method to simulate boundary layer effects by computing the friction velocity, Monin-Obukhov length, surface roughness, and mixing height over the water surface. The details of the formulation of marine dispersion algorithms are provided in the documentation accompanying the CALPUFF modeling system.

To perform its simulation of the coastal environment, CALMET requires hourly observations of air temperature, air-sea temperature difference, wind speed and direction, relative humidity, overwater mixing height, and the overwater temperature gradients above and below the overwater mixing height. For practical applications of overwater boundary layer computations, these data can be obtained from the National Data Buoy Center (NBDC). The NBDC maintains an inventory of standard meteorological data observed by ships, buoys, and C-MAN stations in coastal, near-shore, and offshore locations. NDBC's data sets provide direct wind and temperature measurements, and relative humidity can be inferred from pressure and dewpoint observations. The mixing height and temperature gradients and default values must be applied by CALMET when simulating the coastal atmosphere.

In refined analyses for Honeywell's BART applicability modeling analysis (if necessary), overwater data would be provided in addition to the hourly surface meteorological observations, precipitation observations, and twice-daily upper air sounding data due to the location of the Swanquarter Class I area on the Atlantic coastline.

3.4 AIR QUALITY DATABASE

The CALPUFF model is capable of simulating linear chemical transformation effects by using pseudo-first-order chemical reaction mechanisms for the conversions of SO_2 to SO_4, and NO_X, which consists of nitrogen oxide (NO) and nitrogen dioxide (NO_2), to nitrate (NO_3) and nitric acid (HNO_3). In this study, chemical transformations involving five species (SO_2, SO_4, NO_X, HNO_3, and NO_3) will be modeled using the MESOPUFF II chemical transformation scheme. Ambient concentrations of ammonia and ozone concentrations as represented in the model affect the MESOPUFF II chemical transformation simulation.

3.4.1 OZONE BACKGROUND CONCENTRATIONS

Both screening and refined analyses will utilize observed ozone data for 2001 through 2003 from non-urban CASTNet and AIRS stations compiled by the VISTAS technical contractor for the regional domain. Monthly average ozone background values will be computed based on daytime average ozone concentrations from the OZONE.DAT file (6am-6pm average ozone concentrations computed by month) for substitution should all observations be missing for a particular hour of the dataset.

3.4.2 AMMONIA BACKGROUND CONCENTRATIONS

In the screening and refined analyses, a constant background value (0.5 ppb) for ammonia will be utilized. The *VISTAS BART Modeling Protocol* envisions that CMAQ-modeled NH_3 data for each Class I area would be used during postprocessing of refined analyses to repartition HNO_3 and NO_3 using the ammonia limiting method. However, as of the date of this modeling protocol, the specific values for the five Class I areas considered in Honeywell's modeling analysis have not been specified. Similarly, ammonia boundary conditions and modeled background levels that could be used in the refined CALPUFF analyses have not been provided. Honeywell anticipates additional communication with DEQ as details become available during the time between the modeling protocol submittal and applicability analysis deadline to ensure a mutually agreeable approach for representing ammonia is used in the analyses.

3.4.3 OTHER POLLUTANT BACKGROUND AND BOUNDARY CONDITIONS

The *VISTAS BART Modeling Protocol* envisions the use of modeled boundary conditions of ammonia and sulfates in the refined analysis of chemical transformations involving these species and nitrates. The *VISTAS BART Modeling Protocol* did not provide specific details about these boundary conditions, and as of the data of this source-specific modeling protocol for Honeywell's Hopewell plant, VISTAS has not yet provided this information. Because Honeywell anticipates the possible need to conduct refined analyses for the BART-eligible sources at the Hopewell plant, appropriate boundary conditions will be used in the refined analyses and appropriate documentation will be provided in the BART applicability modeling final report.

3.5 NATURAL CONDITIONS AT CLASS I AREAS

The visibility goal of the Clean Air Act is both the remedying of existing visibility impairment, and prevention of future visibility impairment. In its *BART Implementation Guidance*, U.S. EPA affirms that it interprets the goal to mean return atmospheric conditions to "natural visibility conditions." For the purposes of the Regional Haze Rule program, the U.S. EPA's *Guidance for Estimating Natural Visibility Conditions Under the Regional Haze Rule* and *Guidance for Tracking Progress under the Regional Haze Rule* documents specify the 20% best days at each Class I area as the natural visibility goal.

For the five Class I areas within 300 km of the Hopewell plant and potentially affected by Honeywell's operations, Table 3-1 summarizes the default natural background conditions as tabulated in Appendix B of U.S. EPA's *Guidance for Estimating Natural Visibility Conditions under the Regional Haze Rule*.

TABLE 3-1. NATURAL BACKGROUND CONCENTRATIONS ON 20% BEST DAYS FOR CLASS I AREAS POTENTIALLY AFFECTED BY THE HOPEWELL PLANT

Class I Area	b_{ext} (Mm^{-1})	Annual Average Haze Index (dv)	Best Days Haze Index (dv)	Worst Days Haze Index (dv)
Shenandoah	20.98	7.41	3.57	11.25
James River Face	20.96	7.40	3.56	11.24
Swanquarter	20.91	7.38	3.54	11.22
Dolly Sods	21.13	7.48	3.64	11.32
Otter Creek	21.14	7.49	3.65	11.33

* As tabulated in Appendix B of U.S. EPA's *Guidance for Estimating Natural Visibility Conditions under the Regional Haze Rule* (2003).

To represent natural conditions in the absence of anthropogenic sources of sulfates and nitrates, the monthly background extinction coefficient is expressed in terms of Rayleigh scattering and scattering due to soils (i.e., fine particles) based on the 20% best visibility days, and is calculated from the tabulated "best days" values and the following equations.

$$b_{back} = 10 \exp\left(\frac{HI}{10}\right),$$

where *HI* is Haze Index expressed in units of deciviews (dv). Therefore, total b_{back} for the best days at the five Class I areas, including the Rayleigh scattering coefficient is calculated as shown in the following equations.

$$b_{back} = 10\exp\left(\frac{3.57}{10}\right) = 14.29\ \text{Mm}^{-1} = b_{ray} + b_{soil} = 10\ \text{Mm}^{-1} + b_{soil} \Rightarrow b_{soil} = 4.29\ \text{Mm}^{-1}\ \text{for Shenandoah}$$

$$b_{back} = 10\exp\left(\frac{3.56}{10}\right) = 14.28\ \text{Mm}^{-1} = b_{ray} + b_{soil} = 10\ \text{Mm}^{-1} + b_{soil} \Rightarrow b_{soil} = 4.28\ \text{Mm}^{-1}\ \text{for James River Face}$$

$$b_{back} = 10\exp\left(\frac{3.54}{10}\right) = 14.25\ \text{Mm}^{-1} = b_{ray} + b_{soil} = 10\ \text{Mm}^{-1} + b_{soil} \Rightarrow b_{soil} = 4.25\ \text{Mm}^{-1}\ \text{for Swanquarter}$$

$$b_{back} = 10\exp\left(\frac{3.64}{10}\right) = 14.39\ \text{Mm}^{-1} = b_{ray} + b_{soil} = 10\ \text{Mm}^{-1} + b_{soil} \Rightarrow b_{soil} = 4.39\ \text{Mm}^{-1}\ \text{for Dolly Sods}$$

$$b_{back} = 10\exp\left(\frac{3.76}{10}\right) = 14.41\ \text{Mm}^{-1} = b_{ray} + b_{soil} = 10\ \text{Mm}^{-1} + b_{soil} \Rightarrow b_{soil} = 4.41\ \text{Mm}^{-1}\ \text{for Otter Creek}$$

In its record of revisions to the *VISTAS BART Modeling Protocol*, VISTAS indicates that an unresolved issue as of the date of this modeling protocol is whether U.S. EPA would accept the definition of natural conditions as the annual average of concentrations of visibility-affecting species. If the same approach is used to define the natural background for annual average haze index in terms of soils, the following equations would be used.

$$b_{back} = 10\exp\left(\frac{7.41}{10}\right) = 20.98\ \text{Mm}^{-1} = b_{ray} + b_{soil} = 10\ \text{Mm}^{-1} + b_{soil} \Rightarrow b_{soil} = 10.98\ \text{Mm}^{-1}\ \text{for Shenandoah}$$

$$b_{back} = 10\exp\left(\frac{7.40}{10}\right) = 20.96\ \text{Mm}^{-1} = b_{ray} + b_{soil} = 10\ \text{Mm}^{-1} + b_{soil} \Rightarrow b_{soil} = 10.96\ \text{Mm}^{-1}\ \text{for James River Face}$$

$$b_{back} = 10\exp\left(\frac{7.38}{10}\right) = 20.92\ \text{Mm}^{-1} = b_{ray} + b_{soil} = 10\ \text{Mm}^{-1} + b_{soil} \Rightarrow b_{soil} = 10.92\ \text{Mm}^{-1}\ \text{for Swanquarter}$$

$$b_{back} = 10\exp\left(\frac{7.48}{10}\right) = 21.13\ \text{Mm}^{-1} = b_{ray} + b_{soil} = 10\ \text{Mm}^{-1} + b_{soil} \Rightarrow b_{soil} = 11.13\ \text{Mm}^{-1}\ \text{for Dolly Sods}$$

$$b_{back} = 10\exp\left(\frac{7.49}{10}\right) = 21.14\ \text{Mm}^{-1} = b_{ray} + b_{soil} = 10\ \text{Mm}^{-1} + b_{soil} \Rightarrow b_{soil} = 11.14\ \text{Mm}^{-1}\ \text{for Otter Creek}$$

Alternatively, Table 3-2 summarizes the default natural background conditions using average natural concentrations of sulfate, nitrate, and particulate species for areas in the Eastern U.S. as tabulated in Table 2-1 of U.S. EPA's *Guidance for Estimating Natural Visibility Conditions under the Regional Haze Rule*.

TABLE 3-2. NATURAL BACKGROUND CONCENTRATIONS OF VISIBILITY-AFFECTING POLLUTANTS

Component	West ($\mu g/m^3$)	East ($\mu g/m^3$)	Error Factor	Dry Extinction Efficiency (m^2/g)
Ammonium sulfate	0.12	0.23	2	3
Ammonium nitrate	0.1	0.1	2	3
Organic carbon mass	0.47	1.4	2	4
Elemental carbon	0.02	0.02	2-3	10
Soil	0.5	0.5	1½ - 2	1
Coarse Mass	3	3	1½ - 2	0.6

As is described in Section 4 of this protocol, the effects of relative humidity to amplify the visibility impairment of hygroscopic sulfates and nitrates will be characterized using "Method 6," which computes Δb_{ext} using a *monthly average* relative humidity adjustment particular to each Class I area applied to background and modeled sulfate and nitrate. Table 3-3 summarizes the monthly average humidity values that will be applied for the five Class I areas considered in this analysis, as tabulated in Table A-3 of U.S. EPA's *Guidance for Estimating Natural Visibility Conditions under the Regional Haze Rule*.

TABLE 3-3. MONTHLY AVERAGE *f*(RH) FOR SELECTED CLASS I AREAS*

Class I Area	January	February	March	April	May	June	July	August	September	October	November	December
Shenandoah	3.1	2.8	2.8	2.5	3.1	3.4	3.5	3.9	3.9	3.2	3.0	3.1
James River Face	2.8	2.6	2.7	2.4	3.0	3.3	3.4	3.7	3.6	3.2	2.8	3.0
Swanquarter	2.9	2.7	2.6	2.5	2.9	3.2	3.4	3.5	3.4	3.1	2.8	2.9
Dolly Sods	3.0	2.8	2.8	2.6	3.1	3.4	3.5	3.9	3.9	3.3	3.0	3.1
Otter Creek	3.0	2.8	2.8	2.6	3.2	3.5	3.7	4.1	4.0	3.3	3.0	3.1

* As tabulated in Table A-3 of U.S. EPA's *Guidance for Estimating Natural Visibility Conditions under the Regional Haze Rule* (2003).

Natural background conditions for each Class I area will be calculated using the data summarized in Tables 3-1, 3-2, and 3-3, and the default IMPROVE light extinction formula, which is summarized in the following equation.

$$b_{ext,background}(km^{-1}) = b_{SO_4} + b_{NO_3} + b_{OC} + b_{soil} + b_{coarse} + b_{ap} + b_{ray}$$

where,

$$b_{SO_4} = 0.003\left[(\mathrm{NH_4})_2\mathrm{SO_4}\right]f(RH)$$
$$b_{NO_3} = 0.003\left[\mathrm{NH_4NO_3}\right]f(RH)$$
$$b_{OC} = 0.004\left[\mathrm{OC}\right]$$
$$b_{Soil} = 0.001\left[\mathrm{Soil}\right]$$
$$b_{Coarse} = 0.0006\left[\mathrm{Coarse\ Mass}\right]$$
$$b_{ap} = 0.01[\mathrm{Elemental\ Carbon}]$$
$$\mathrm{b_{Ray}} = \mathrm{Rayleigh\ Scattering}$$
$$\mathrm{f(RH)} = \mathrm{relative\ humidity\ adjustment\ factor}$$
$$[\quad] = \mathrm{Concentration\ in\ \mu g/m^3}$$

As noted in the *VISTAS BART Modeling Protocol*, the U.S. EPA and the Regional Planning Organizations (including VISTAS) are evaluating whether refinements are warranted to the methods recommended in U.S. EPA's guidance to calculate default estimates of natural background visibility. In addition, the Interagency Monitoring of Protected Visual Environments (IMPROVE) work group has recently approved an alternative to the default formula used to estimate extinction from particle concentration measurements.[11] Refinements in the revised IMPROVE formula include the following:

- Adding a sea salt term, including a growth factor due to relative humidity
- Increasing the factor used to calculate the mass of particulate organic matter from organic carbon measurements
- Modifying the relative humidity growth formula, *f*(RH), for sulfates and nitrates
- Revising the extinction efficiencies (the numerical constants in Equation 3-1) for sulfates, nitrates, and organic carbon so that they vary with concentration
- Adding a site-specific Rayleigh scattering term to the formula. Values will be calculated by IMPROVE for all Class I areas.

For the purposes of calculating current, future, and natural background visibility at Class I areas as part of its reasonable progress analyses, VISTAS intends to present regional air quality modeling results using both the current U.S. EPA recommended assumptions and the newly revised IMPROVE light extinction formula. Accordingly, in any refined BART applicability analyses that may be required, Honeywell may evaluate the results of the analysis using both formulas as well as appropriate refinements (e.g., sea salt and Rayleigh scattering correction) to assess the frequency, duration, and magnitude of visibility impairment events.

[11] Pitchford, M., W. Malm, B. Schichtel, N. Kumar, D. Lowenthal, and J. Hand, 2005. *Revised IMPROVE Algorithm for Estimating Light Extinction from Particle Speciation Data*. Report to IMPROVE Steering Committee, November 2005.

4. AIR QUALITY MODELING METHODOLOGY

Section 4 of this BART applicability modeling protocol for Honeywell's Hopewell plant describes the air quality modeling methodology that will be used in the screening and refined analyses. The information in this Section 4 is largely adapted from the *VISTAS BART Modeling Protocol*, which is presented in Appendix A of this source-specific protocol for reference, and sample model files made available on the VISTAS technical contractor website.[12]

Section 2.2 of the *VISTAS BART Modeling Protocol* summarizes recommendations for the air quality modeling analyses required to assess applicability of BART by determining whether Honeywell's Hopewell plant contributes to visibility impairment at Class I areas within 300 km, which include Shenandoah NP (158 km), James River Face WA (190 km), Swanquarter NWR (227 km), Dolly Sods WA (258 km) and Otter Creek WA (275 km). The CALPUFF modeling system is recommended as the preferred modeling approach for use in the BART analyses.

4.1 PLUME MODEL SELECTION

CALPUFF and its meteorological model, CALMET, are designed to handle the complexities posed by the complex terrain, the large source-receptor distances, chemical transformation and deposition, and other issues related to Class I visibility impacts. The CALPUFF modeling system has been adopted by the U.S. EPA as a *Guideline* model for source-receptor distances greater than 50 km, and for use on a case-by-case basis in complex flow situations for shorter distances. CALPUFF is recommended for Class I impact assessments by FLAG and IWAQM. The final BART guidance recommends CALPUFF as "the best modeling application available for predicting a singe source's contribution to visibility impairment." As a result of these recommendations, the *VISTAS BART Modeling Protocol* is based on the use of CALPUFF for its BART determinations. Specifically, VISTAS CALMET Version 5.7 and CALPUFF Version 5.8 will be used in the CALPUFF analyses for BART applicability assessment, or other appropriate versions as specified by VISTAS and it technical contractor.[13]

This source-specific modeling protocol for Honeywell's Hopewell plant incorporates by reference the *VISTAS BART Modeling Protocol*, which is provided in Appendix A of this document. The following sections present a brief summary of major features of the CALMET and CALPUFF models, and further detailed information should be obtained from the *VISTAS BART Modeling Protocol* and documentation referenced therein.

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[12] http://src.com/verio/download/download.htm#VISTAS_VERSION.

[13] Although the *VISTAS BART Modeling Protocol* specifies CALMET Version 5.7 and CALPUFF Version 5.8, as of the date of this modeling protocol, the technical contractor website maintains CALPUFF Version 5.754 and CALMET Version 5.711.

4.1.1 MAJOR RELEVANT FEATURES OF CALMET

The CALMET meteorological model consists of a diagnostic wind field module and boundary layer micrometeorological modules for overwater and overland boundary layers. Over land surfaces, the energy balance method of Holtslag and van Ulden (1983) is used to compute hourly gridded fields of the sensible heat flux, surface friction velocity, Monin-Obukhov length, and convective velocity scale. Mixing heights are determined from the computed hourly surface heat fluxes and observed temperature soundings using a modified Carson (1973) method based on Maul (1980). The model also determines gridded fields of Pasquill-Gifford-Turner (PGT) stability class and hourly precipitation rates.

The aerodynamic and thermal properties of water surfaces suggest that a different method is best suited for calculating the boundary layer parameters in the marine environment. A profile technique, using air-sea temperature differences, is used in CALMET to compute the micro-meteorological parameters in the marine boundary layer. The version of CALMET being used by VISTAS contains improvements in the overwater boundary layer parameterizations (Fairall et al., 2003) based on the Coupled Ocean Atmosphere Response Experiment (COARE) and enhancements in the calculation of overwater mixed layer heights (Batchvarova and Gryning, 1991, 1994). Further details and the results of an evaluation of the model containing these enhancements are described in Scire et al. (2005). An upwind-looking spatial averaging scheme is optionally applied to the mixing heights and three-dimensional temperature fields in order to account for important advective effects.

The diagnostic wind field module uses a two-step approach to the computation of the wind fields (Douglas and Kessler, 1988). In the first step, an initial-guess wind field is adjusted for kinematic effects of terrain, slope flows, and terrain blocking effects to produce a Step 1 wind field. Gridded MM5 can be used to define the initial guess field. The second step consists of an objective analysis procedure to introduce observational data into the Step 1 wind field to produce a final wind field.

Development of the Step 1 wind field begins with the initial guess field defined by the MM5 prognostic meteorological model. Normally, the CALMET computational domain is specified to be at finer grid resolution than the MM5 dataset used to initialize the initial guess field. For example, 36-km MM5 data available for VISTAS modeling may be used to develop the initial guess field on a 12-km or even a 1-km CALMET grid. The Step 1 algorithms in CALMET described below apply terrain adjustments to the initial guess field on the fine-scale CALMET grid. Thus, the CALMET winds are adjusted to respond to fine-scale terrain features not necessarily seen by the coarser scale MM5 model.

The approach of Liu and Yocke (1980) is used to evaluate the effects of the kinematic terrain on the wind field. The initial guess field winds are used to compute a terrain-forced vertical velocity, subject to an exponential, stability-dependent decay function. The effects of terrain on the horizontal wind components are evaluated by applying a divergence-minimization scheme to the initial guess wind field. The divergence minimization scheme is applied iteratively until the three-dimensional divergence is less than a threshold value.

The original slope flow algorithm in CALMET has been upgraded (Scire and Robe, 1997) based on the shooting flow algorithm of Mahrt (1982). This scheme includes both advective-gravity and equilibrium flow regimes. At night, the slope flow model parameterizes the flow down the sides of the valley walls into the floor of the valley, and during the day, upslope flows are parameterized. The magnitude of the slope flow depends on the local surface sensible heat flux and local terrain gradients. The slope flow wind components are added to the wind field adjusted for kinematic effects.

The thermodynamic blocking effects of terrain on the wind flow are parameterized in terms of the local Froude number (Allwine and Whiteman, 1985). If the Froude number at a particular grid point is less than a critical value and the wind has an uphill component, the wind direction is adjusted to be tangent to the terrain.

The wind field resulting from the preceding adjustments of the initial-guess wind is the Step 1 wind field. The second step of the procedure may involve introduction of observational data into the Step 1 wind field through an objective analysis procedure. An inverse-distance squared interpolation scheme is used which weights observational data heavily in the vicinity of the observational station, while the Step 1 wind field dominates the interpolated wind field in regions with no observational data. The resulting wind field is subject to smoothing, an optional adjustment of vertical velocities based on the O'Brien (1970) method, and divergence minimization to produce a final Step 2 wind field.

The introduction of observational data in the Step 2 calculation is an option. It is also possible to run the model in "no observations" (No-Obs) mode, which involves the use only of MM5 gridded data for the initial guess field followed by fine-scale terrain adjustments by CALMET. In No-Obs mode, observational data are not used in the Step 2 calculations. The No-Obs mode is appropriate when the MM5 simulations adequately characterize the regional wind patterns and when local observations, especially surface observations, reflect local conditions on a scale smaller than that of the CALMET domain and hence their spatial representativeness may be limited. Such situations are most likely to occur when the CALMET grid scale is relatively large i.e., coarser than the scale of variation of the true wind field, which is particularly likely to occur in complex terrain or along the seashore.

As was described in Section 3.1.1 of this protocol, when the 12-km MM5 (2001 and 2002) data are used, the diagnostic CALMET terrain adjustments were turned off since the grid resolution of the MM5 data is the same as the CALMET grid and the terrain adjustments on the 12-km grid scale will already be reflected in the MM5 dataset. In this case, the MM5 winds will be interpolated by CALMET to the CALMET layers and CALMET's boundary layer modules will compute mixing heights, turbulence parameters and other meteorological parameters that are required by CALPUFF. For 2003, the 36-km MM5 data were used as CALMET's initial guess field and then the CALMET diagnostic terrain adjustments (see Section 3.1.1 of the *VISTAS BART Modeling Protocol*) were applied to reflect terrain on the scale of the CALMET grid (i.e., 12 km). Refined analyses, if required, will utilize the MM5 data as the first-guess wind field, apply the diagnostic algorithms to create the Step 1 winds, and use NWS data for smoothing in Step 2.

4.1.2 MAJOR RELEVANT FEATURES OF CALPUFF

By its puff-based formulation and through the use of three-dimensional meteorological data developed by the CALMET meteorological model, CALPUFF can simulate the effects of time- and space-varying meteorological conditions on pollutant transport from sources in complex terrain. The major features and options of the CALPUFF model are summarized in Table 3-2 of the *VISTAS BART Modeling Protocol*. Some of the technical algorithms are briefly described as follows.

- Complex Terrain: The effects of complex terrain on puff transport are derived from the CALMET winds. In addition, puff-terrain interactions at gridded and discrete receptor locations are simulated using one of two algorithms that modify the puff-height (either that of ISCST3 or a general "plume path coefficient" adjustment), or an algorithm that simulates enhanced vertical dispersion derived from the weakly-stratified flow and dispersion module of the Complex Terrain Dispersion Model (CTDMPLUS) (Perry et al., 1989). The puff-height adjustment algorithms rely on the receptor elevation (relative to the elevation at the source) and the height of the puff above the surface. The enhanced dispersion adjustment relies on the slope of the gridded terrain in the direction of transport during the time step.
- Subgrid Scale Complex Terrain (CTSG): An optional module in CALPUFF, CTSG treats terrain features that are not resolved by the gridded terrain field, and is based on the CTDMPLUS (Perry et al., 1989). Plume impingement on subgrid-scale hills is evaluated at the CTSG subgroup of receptors using a dividing streamline height (H_d) to determine which pollutant material is deflected around the sides of a hill (below H_d) and which material is advected over the hill (above H_d). The local flow (near the feature) used to define H_d is taken from the gridded CALMET fields. As in CTDMPLUS, each feature is modeled in isolation with its own set of receptors.
- Puff Sampling Functions: A set of accurate and computationally efficient puff sampling routines is included in CALPUFF, which solve many of the computational difficulties encountered when applying a puff model to near-field releases. For near-field applications during rapidly-varying meteorological conditions, an elongated puff (slug) sampling function may be used. An integrated puff approach may be used during less demanding conditions. Both techniques reproduce continuous plume results under the appropriate steady state conditions.
- Building Downwash: The Huber-Snyder and Schulman-Scire downwash models are both incorporated into CALPUFF. An option is provided to use either model for all stacks, or make the choice on a stack-by-stack and wind sector-by-wind sector basis. Both algorithms have been implemented in such a way as to allow the use of wind direction specific building dimensions. The PRIME building downwash model (Schulman et al., 2000) is also included in CALPUFF as an option.
- Dispersion Coefficients: Several options are provided in CALPUFF for the computation of dispersion coefficients, including the use of turbulence measurements (σ_v and σ_w), the use of similarity theory to estimate σ_v and σ_w from modeled surface

heat and momentum fluxes, or the use of Pasquill-Gifford (PG) or McElroy-Pooler (MP) dispersion coefficients, or dispersion equations based on the CTDM. Options are provided to apply an averaging time correction or surface roughness length adjustments to the PG coefficients. In Version 5.8 of CALPUFF being used by VISTAS, an option is provided to use the AERMOD turbulence profiles for determining dispersion rates, which is the most recent approach to dispersion in EPA-approved regulatory modeling. In addition, turbulence advection is included. For additional details on these features, see Scire et al. (2005).

- ▲ Overwater and Coastal Interaction Effects: Because the CALMET meteorological model contains both overwater and overland boundary layer algorithms, the effects of water bodies on plume transport, dispersion, and deposition can be simulated with CALPUFF. The puff formulation of CALPUFF is designed to handle spatial changes in meteorological and dispersion conditions, including the abrupt changes that occur at the coastline of a major body of water.
- ▲ Dry Deposition: A resistance model is provided in CALPUFF for the computation of dry deposition rates of gases and particulate matter as a function of geophysical parameters, meteorological conditions, and pollutant species. For particles, source-specific mass distributions may be provided for use in the resistance model. Of particular interest for BART analyses is the ability to separately model the deposition of fine particulate matter (< 2.5 μm diameter) from coarse particulate matter (2.5-10 μm diameter).
- ▲ Wind Shear Effects: CALPUFF contains an optional puff splitting algorithm that allows vertical wind shear effects across individual puffs to be simulated. Differential rates of dispersion and transport among the "new" puffs generated from the original, well-mixed puff can substantially increase the effective rate of horizontal spread of the material. Puffs may also be split in the horizontal when the puff size becomes large relative to the grid size, to account for wind shear across the puffs.
- ▲ Wet Deposition: An empirical scavenging coefficient approach is used in CALPUFF to compute the depletion and wet deposition fluxes due to precipitation scavenging. The scavenging coefficients are specified as a function of the pollutant and precipitation type (i.e., frozen vs. liquid precipitation).
- ▲ Chemical Transformation: CALPUFF includes options for parameterizing chemical transformation effects using the five species scheme (SO_2, $SO_4^{=}$, NO_X, HNO_3, and NO_3^-) employed in the MESOPUFF II model or a set of user-specified, diurnally-varying transformation rates. The MESOPUFF II scheme is recommended by IWAQM. It produces secondary fine particulate matter (sulfate and nitrate) from emissions of SO_2 and NO_X and thus allows analyses of visibility impacts. Ambient ozone concentrations are used in the parameterized chemical transformation module as a surrogate for OH radicals during daylight hours. Ambient ammonia concentrations are used together with a temperature and relative humidity-dependent equilibrium relationship to partition nitric acid and nitrate on an hour-by-hour and receptor-by-receptor basis.

4.2 MODELING DOMAIN CONFIGURATION

The VISTAS regional modeling domain was illustrated in Figure 3-1 in the preceding section of this protocol, and was designed to allow any Class I areas within the VISTAS area to be evaluated with a single meteorological database and consistent CALPUFF modeling options. The horizontal domain is comprised of grid cells, each containing a central grid point at which meteorological and computational parameters are calculated at each time step. For the initial regional analysis, a grid spacing interval of 12 km was selected. Given this interval, the domain consists of 160 by 172 grid cells. A Lambert Conformal Coordinate projection system is used to describe the horizontal grid, with origin at 40 degrees North latitude and 97 degrees West longitude. Standard parallels for the projection were set at 33 degrees North and 45 degrees North.

Table 4-1 summarizes the vertical grid structure selected for this analysis, which comprises ten vertical layers. The cell face height of each layer indicates its vertical extent. The vertical domain is composed of terrain-following grid cells, the number and size of which are chosen so as to constrain the boundary layer in which dispersion and chemical transformations take place. The highest cell face was selected to be 4,000 meters to constrain the default maximum mixing height of 3,000 meters.

TABLE 4-1. VERTICAL GRID STRUCTURE

Vertical Grid Cell	Cell Face Height (meters)
1	20
2	40
3	80
4	160
5	320
6	640
7	1,200
8	2,000
9	3,000
10	4,000

Refined analyses, if necessary, will be conducted using one or more of the subregional 4-km grids that the VISTAS technical contractor will provide. Honeywell anticipates that refined analyses may be necessary for either or both of the Class I areas, in which case the appropriate subregional grid would be utilized. Additional runs at higher resolution (e.g., 1 km) may be performed and the modeling subdomain would be selected appropriately from the VISTAS regional grid.

4.3 CALMET METEOROLOGICAL MODELING

CALMET meteorological modeling for the initial regional screening analysis was conducted over the entire VISTAS regional domain described in section 4.2. The major features of CALMET were described in Section 4.1.1 of this protocol, and the geophysical and meteorological databases were described in Section 3. CALMET processing was conducted generally in accordance with the recommendations of IWAQM *Phase 2 Summary Report and Recommendations for Modeling Long Range Transport Impacts*, with the following exceptions and/or specifications of non-default values.

- ▲ Modeling period: 2001 through 2003
- ▲ Meteorological inputs: MM5 data provide initial guess fields in CALMET
- ▲ CALMET mode: No-Observations mode including option to read overwater data directly from MM5
- ▲ Diagnostic options: IWAQM default values, except as follows: diagnostic terrain blocking and slope flow algorithms used for 2003 simulations (using 36-km MM5 data), but no diagnostic terrain adjustments in 2001 and 2002 simulation (using 12-km MM5 data)
- ▲ CALMET options dealing with radius of influence parameters (R1, R2, RMAX1, RMAX2, RMAX3), BIAS, ICALM parameters are not used in No-Observations mode.
- ▲ TERRAD (terrain scale) is required for runs with diagnostic terrain adjustments (i.e., the 2003 simulations). Values of ~10-20 km were tested, and a value of 15 km was selected by the VISTAS technical contractor.
- ▲ Land use defining water: JWAT1 = 55, JWAT2 = 55 (large bodies of water). This feature allows the temperature field over large bodies of water such as the Atlantic Ocean and the Great Lakes to be properly characterized by buoy observations.
- ▲ Mixing height averaging parameter (MNMDAV) was determined by the VISTAS technical contractor to be 1 grid cell for regional simulations based on sensitivity tests. The purpose of the testing was to optimize the variable to allow spatial variability in the mixing height field, but without excessive noise.

Refined analyses, if necessary, will be prepared using appropriate CALMET model settings as described by the VISTAS technical contractor for the 4 km subregional grids utilized. Should even higher resolution (e.g., 1 km) analyses be conducted, appropriate CALMET processing options will be evaluated and documented in the final applicability modeling report.

4.4 CALPUFF COMPUTATIONAL DOMAIN AND RECEPTORS

CALPUFF analyses to assess the visibility impacts attributable to Honeywell's Hopewell plant will be performed on a computational domain that is a subset of the VISTAS regional domain. The size of the domain will be selected to encompass the Hopewell plant and the five Class I areas, and to extend at least 50 km beyond in all directions. The size of the domain allows for the possible recirculation of puffs beyond the facility and areas being evaluated. Ambient impacts will be predicted at receptors specified by the FLM to represent the five Class I areas as depicted in Figure 1-2 of this protocol.[14]

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[14] http://www2.nature.nps.gov/air/maps/Receptors/index.htm

4.5 CALPUFF MODELING OPTION SELECTIONS

The CALPUFF analysis will be conducted generally in accordance with the recommendations of IWAQM *Phase 2 Summary Report and Recommendations for Modeling Long Range Transport Impacts*, with the following exceptions and/or specifications of non-default values.

- ▲ Chemical mechanism: MESOPUFF II module
- ▲ Background concentrations of SO_4 and TNO_3 ($HNO_3 + NO_3$) from CMAQ 2001-2003 annual runs. Note that as of the date of this protocol, the appropriate background levels for each Class I area have not yet been specified. **Honeywell requests that DEQ confirm the appropriate values in response to this modeling protocol should refined modeling be necessary.**
- ▲ Species modeled: SO_2, SO_4, NO_X, HNO_3, NO_3 and particulate matter in size categories of <0.625 µm, 0.625-1.0 µm, 1.0-1.25 µm, 1.25-2.5 µm, 2.5-6.0 µm and 6-10 µm aerodynamic diameters. Because Honeywell's BART-eligible source comprises more than one emission point, emissions of each particle type (i.e., PIC, POC, PMC, PMF, and EC) will be explicitly modeled.
- ▲ Emission rates for modeling based on U.S. EPA BART guidance, i.e., maximum 24-hour actual emission rate with normal operations from the highest emitting day of the meteorological period modeled (excluding days where start-up, shutdown or malfunctions occurred sometime during the day). Note that potential emissions are used to determine if a source is BART-eligible, but 24-hour average maximum emissions are used for modeling purposes (70 FR 39162). Pollutants considered include SO_2, H_2SO_4, NO_X and PM_{10}. The basis for modeled emission rates was described in Section 2 of this protocol.
- ▲ Condensable emissions are considered as primary fine particulate matter and allocated equally to the two sub-micrometer particle size classes. Industry-specific emission factors were utilized to analyze the phase, size, and character of PM emissions as described in Section 2 of this protocol.
- ▲ Excluded from the modeling are pollutants with plant-wide emissions less than *de minimis* levels (40 tons per year for SO_2 and NO_X and 15 tons per year for PM_{10}). *De minimis* levels are plant wide for each visibility-impairing pollutant, so individual units may be modeled even if they have emissions below *de minimis* if the plant total is greater than *de minimis*. Per DEQ guidance, Honeywell further excluded otherwise BART-eligible emission units that emit NO_X, SO_2, and PM_{10} in amounts less than the Title V *de minimis* level (5 tpy).
- ▲ Particulate emissions speciation: Break down, as appropriate, filterable and condensable particulate matter into the following species categories: elemental carbon (soot), "soil" (fine PM < 2.5 µm diameter), coarse particulate matter (2.5-10 µm diameter) and organics. Industry-specific emission factors were utilized to analyze the phase, size, and character of PM emissions as described in Section 2 of this protocol.
- ▲ CALPUFF model options: Use IWAQM guidance, including Pasquill-Gifford (ISC-like) dispersion coefficients. The use of turbulence-based dispersion coefficients and probability density function (pdf) dispersion, as used in the AERMOD model, will be evaluated should refined modeling analyses be necessary.

- Ozone dataset: use observed ozone data for 2001 through 2003 from CASTNet and AIRS stations. Only non-urban ozone stations should be used in the OZONE.DAT file. Monthly average ozone (backup) background values are to be computed based on daytime average ozone concentrations from the OZONE.DAT file (6am-6pm average ozone concentrations computed by month).
- Background ammonia concentration: In CALPUFF, use constant (0.5 ppb) values for ammonia. CMAQ NH_3 data will be used for each Class I area in POSTUTIL to repartition HNO_3 and NO_3. Note that as of the date of this protocol, the appropriate background levels for each Class I area have not yet been specified. **Honeywell requests that DEQ confirm the appropriate values in response to this modeling protocol.**
- Puff representation: integrated puff sampling methodology.
- Building downwash: Since the nearest Class I area is located more than 250 km to the facility, effects of building downwash will not be evaluated.

4.6 CALPOST PROCESSING OPTION SELECTIONS FOR LIGHT EXTINCTION AND HAZE IMPACT CALCULATIONS

The following postprocessing techniques will be used to compute the 24-hour average visibility impacts at each Class I area within 300 km of Honeywell's Hopewell plant.

- Species considered in visibility analysis: SO_4, NO_3, EC, SOA (i.e., condensable organic emissions), soil (fine filterable PM), coarse PM
- Visibility Method 6 will be used with Class I area-specific, monthly average, relative humidity values as described in Section 3.5 of this protocol.
- Natural background light extinction will be represented at each Class I area within 300 km of Honeywell's Hopewell plant as described in Section 3.5 of this protocol using both the 20% best days and annual average natural concentrations of visibility-affecting pollutants.
- Light extinction efficiencies: Use EPA (2003a) values. Honeywell will evaluate the use of the 2005 IMPROVE algorithm for calculating light extinction, which the *VISTAS BART Modeling Protocol* indicates may be used in addition to the default IMPROVE algorithm. Calculations would be performed outside CALPOST unless CALPOST is modified to accommodate the new algorithm. Scattering efficiencies for sea salt and altitude-dependent Rayleigh scattering corrections will be evaluated for use in both the default and revised IMPROVE calculations.
- Ammonia Limiting Method: Refined analyses (if necessary) would use ammonia from CMAQ to define NH_3 for each Class I area. Choose ammonia from either the CMAQ grid cell where the IMPROVE monitor is located or the grid cell of the centroid of the Class I area (the latter in the case that the IMPROVE monitor is located outside the Class I area or there is no IMPROVE monitor.)

The initial run results will be based on the highest change in light extinction (deciviews) from natural conditions over the three-year modeling period for each Class I area considered. Predicted changes exceeding the "contribution" threshold (0.5 deciviews) will trigger a finer grid CALPUFF modeling analysis. To assess whether BART-eligible operations contribute to visibility impairment, Honeywell's applicability modeling analysis will demonstrate the top eight 24-hour average visibility impacts of each year modeled to illustrate the distribution (i.e., frequency, duration, and magnitude) of peak visibility impairment episodes attributable to the Hopewell plant. Only the 98th percentile 24-hour average visibility impact would be evaluated in the refined analysis, if necessary.

4.7 MODELING PRODUCTS

Honeywell will prepare and submit a BART applicability analysis result describing the modeling procedures, data resources, and results of screening and refined modeling (if necessary) used to assess whether the Hopewell plant is subject to BART. The presentation of modeling results will generally conform to the expectations described in the *VISTAS BART Modeling Protocol* and described as follows. The results section of the CALPUFF modeling report will contain the following information:

1. Map of source location and Class I areas within 300 km of the source
2. For the VISTAS 12-km CALPUFF initial exemption modeling domain, a table listing all Class I areas in the VISTAS domain and those in neighboring states and impacts at those Class I areas within 300 km of the source
3. A discussion of the number of Class I areas with visibility impairment from the source on 98th percentile days in each year greater than 0.5 dv (total visibility impairment minus impairment on 20% best days for natural background visibility equals delta-dv, the visibility impact attributed to the source).
4. For the Class I area with the maximum impact, discussion of the number of days below the 98th percentile that the impact of the source exceeds 0.5 dv, the number of receptors in the Class I area where the impact exceeds 0.5 dv, and the maximum impact.
5. For finer grid CALPUFF exemption modeling, results for those Class I areas for which impacts of the source exceeded 0.5 dv in the 12-km initial exemption modeling. Report same results as provided for 12-km initial exemption modeling.

5. QUALITY ASSURANCE METHODS

Honeywell will conduct quality assurance of CALMET, CALPUFF, and CALPOST analyses in a manner that generally conforms to the *VISTAS BART Modeling Protocol*. A description of the quality assurance methods and products (e.g., test case simulations, graphic representations of model fields and performance) will be provided in Honeywell's BART Applicability Modeling Report.
The following sections describe techniques that can be used to visualize and quality assure performance of each model component as described in the VISTAS *BART Modeling Protocol*.

5.1 CALMET FIELDS

Section 4 of the *VISTAS BART Modeling Protocol* describes the methods and procedures for use in conducting regional scale screening modeling to determine the whether a particular source or group of sources is subject to BART controls. In the initial application, the regional CALPUFF-ready meteorological data files will be provided by VISTAS. The amount of effort for end-users performing QA of these pre-defined meteorological fields will be reduced from what is required in developing source-specific meteorological fields, as described below. Also, VISTAS is planning to provide five sub-regional CALMET meteorological datasets in a CALPUFF-ready format. The development of these CALMET datasets will be subject to a QA program as part of their development, so the necessary quality assurance activity of end-users is again reduced from what would be required in the development of the dataset. It is not expected that the quality assurance steps in the development will be repeated in each application. The VISTAS-provided regional and sub-regional meteorological fields will include a test case simulation for demonstrating that expected modeling results are obtained on the user's computer platform. Honeywell will execute this test case simulation to demonstrate that the expected results can be reproduced.

The critical CALMET input parameters depend on the mode in which the model is run (i.e., observations mode, hybrid mode, or no-observations mode), and the location and spatial representativeness of any observational data. In a site-specific protocol involving the development of a meteorological dataset, the elements of the QA process include preparation of wind rose (using observed, MM5 and CALMET-derived data), including examination of the data as a function of season and time of day (e.g., 4am, 10am, 4pm wind roses), time series analyses, and presentation of 2-D vector plots illustrating terrain effects/sea breeze circulation or other features of the flow expected to occur within the domain. For example, 2-D vector plots produced during light wind speed stable conditions (e.g., early morning such as 4 am) are good for assessing the performance of the CALMET model configuration and switches in reproducing terrain effects because these conditions are likely to maximize the terrain impacts in the model. Season wind roses at 4 am, 10 am and 4 pm would be expected to show the development of sea breeze circulations that may be important for certain applications. Customization of the QA process for the individual site-specific domain based on the availability of data and the physical processes expected to be important at that location will be conducted as part of the site-specific QA plan development.

5.2 CALPUFF, CALPOST, AND POSTUTIL RESULTS

Most of the CALPUFF input variables contain default values. Appendix B of the IWAQM report contains a list of recommended CALPUFF switch settings. Except as modified in Chapter 4 of the *VISTAS BART Modeling Protocol* or in a source-specific protocol, the IWAQM guidance should be used in setting up the CALPUFF simulations. The CALPUFF model obtains the switch settings from an ASCII "control file" with a default name called the CALPUFF.INP file. As is the case with the comparable CALMET file, it is essential that the control file be reviewed manually as part of the CALPUFF QA analysis. To facilitate this process, as was the case with the CALMET GUI, the CALPUFF GUI retains all of the input descriptive information that is part of the standard CALPUFF.INP file structure.

CALPOST is run separately for each Class I area in order to obtain the necessary visibility statistics for evaluating compliance with the BART screening and finer grid modeling thresholds. The inputs to CALPOST involve selection of the visibility method (Method 6 in the standard U.S EPA BART guidance), entry of Class I area-specific data for computing background extinction and monthly relative humidity factors for hygroscopic aerosols. CALPOST contains a receptor screening that allow subsets of a receptor network modeling in CALPUFF to be selected for processing in a given CALPOST run. This is how receptors within a single Class I area are selected for processing from a CALPUFF output file that may contain receptors from several Class I areas. CALPOST contains options for creating plot files that will help in the confirmation that the proper receptor subset is extracted.

The CALPOST output file contains a listing of the highest visibility impact each day of the model simulation over all receptors included in CALPOST analysis. Receptors will normally be selected in each CALPOST run so that each CALPOST run represents the impacts at a single Class I area. For a screening assessment, the peak value of the change in extinction is shown at the bottom of the visibility table. For a finer grid simulation, the 98th percentile value (8th highest day) is used for comparison against the BART threshold of 0.5 deciviews. It is necessary to import the results of the CALPOST table into a sorting program such as a spreadsheet to rank the daily change in extinction values such as is presented in Table 4-2.

The CALPOST inputs that will be carefully checked as part of the CALPOST quality assurance include the following:

- ▲ Visibility technique (Method 6)
- ▲ Monthly Class I-specific relative humidity factors for Method 6
- ▲ Background light extinction values
- ▲ Inclusion of all appropriate species from modeled sources (e.g., sulfate, nitrate, organics), coarse and fine particulate matter, and elemental carbon.
- ▲ Appropriate species names for coarse PM used
- ▲ Extinction efficiencies for each species
- ▲ Appropriate Rayleigh scattering term (10 Mm^{-1} for screening modeling but Class I area specific value for finer grid modeling)
- ▲ Screen to select appropriate Class I receptors for each CALPOST simulation.

POSTUTIL allows the user to sum the contributions of sources from different CALPUFF simulations into a total concentration file. In addition, it contains options to scale the concentrations from different modeled species (e.g., different particle sizes) into species-dependent size distributions for the particulate matter. For example, PM is often simulated with unit emission rates for each particle size category and, in the POSTUTIL stage, the contributions of each size category based on the species being considered (e.g., elemental carbon, coarse particulate matter, etc.) are combined to form the species concentrations for input into CALPOST. This process, although simple, requires a careful review of the weighting factors for each source. POSTUTIL also allows a repartitioning of nitric acid and nitrate to account for the effects of ammonia limiting conditions.

If site-specific CALPUFF simulations involving the Ammonia Limiting Method are conducted, performance of the model in reproducing observed CASTNet or IMPROVE sulfate and nitrate concentrations at measurement sites within the site-specific modeling domain should be evaluated. The use of alternative ammonia concentration data (e.g., CMAQ output rather than derived ammonia based on aerosol measurements) will require an evaluation of the model performance relative to the techniques in the VISTAS common protocol.

6. REFERENCES

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APPENDIX A

VISTAS BART MODELING PROTOCOL

Protocol for the Application of the CALPUFF Model for Analyses of Best Available Retrofit Technology (BART)

December 22, 2005

(Revision 2 – 3/9/06)

Visibility Improvement State and Tribal Association of the Southeast (VISTAS)

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SUMMARY

This Protocol for the Application of the CALPUFF Model for Analyses of Best Available Retrofit Technology (BART) for the VISTAS Regional Planning Organization (RPO) describes common procedures for carrying out air quality modeling to support BART determinations that are consistent with guidelines of the U.S. Environmental Protection Agency in 40 CFR Part 51 Appendix W and Appendix Y. The Protocol is intended to serve as the basis for a common understanding among the organizations that will be performing BART analyses or reviewing the BART modeling results in the VISTAS region.

Background

Best Available Retrofit Technology is required for any BART-eligible source that ‘‘emits any air pollutant which may reasonably be anticipated to cause or contribute to any impairment of visibility” in any mandatory Class I federal area. According to 40 CFR Part 51 Appendix Y, “*You can use dispersion modeling to determine that an individual source cannot reasonably be anticipated to cause or contribute to visibility impairment in a Class I area and thus is not subject to BART*.” In the “individual source attribution approach,” a BART-eligible source that is responsible for a 1.0 deciview (dv) change or more is considered to “cause” visibility impairment. A BART-eligible source that is responsible for a 0.5 dv change or more is considered to “contribute” to visibility impairment in a Class I area. Any source determined to cause or contribute to visibility impairment in any Class I area is subject to BART.

The member states of the VISTAS RPO agreed to develop a common BART Modeling Protocol to guide them, their sources, and reviewers in the BART determination and review effort. The Protocol has been in preparation within VISTAS since January 2005. The original authors are Pat Brewer, VISTAS Technical Coordinator, and Ivar Tombach, VISTAS Technical Advisor. The VISTAS state BART contacts, particularly Tom Rogers, FL, Chris Arrington, WV, Leigh Bacon, AL, and Michael Kiss, VA, have directed and extensively reviewed the Protocol. The Protocol was enhanced and completed with the assistance of Joseph Scire, Christelle Escoffier-Czaja and Jelena Popovic of Earth Tech, Inc. and it has received extensive contributions and review from the VISTAS federal partners: Federal Land Managers and USEPA. The VISTAS RPO held a meeting on September 21, 2005 in Research Triangle Park, NC to discuss the Protocol with participants before starting a public comment period. The Protocol underwent formal external review during the period between September 26, 2005 and October 31, 2005. Numerous comments were received. All comments were carefully considered and discussed with VISTAS participants and federal partners. VISTAS gratefully acknowledges the very useful contributions of those that provided comments. On November 1st, 2005 VISTAS held another meeting with its participants in Nashville, TN to present and discuss the comments being considered for inclusion in the Protocol. No formal document will be prepared to address all the comments received on the Protocol.

Objectives

The objectives of the Protocol (discussed in Chapter 1) are to provide:

- A consistent approach to determine if a source is subject to BART
- A consistent model (CALPUFF) and modeling guidelines for BART determinations
- Clearly delineated modeling steps
- A common CALPUFF configuration
- Guidance for site-specific modeling
- Common expectations for reporting model results

The Protocol is not intended to define the engineering analyses required by the USEPA BART Guidance, nor address model alternatives to the CALPUFF model, nor address emissions trading.

Chapter 2 is intended to provide summary background on EPA's guidance for BART modeling. The CALPUFF model system is reviewed in Chapter 3, while specific recommendations for applying the CALPUFF model for BART purposes appear in Chapter 4. Chapter 5 describes the specific information that should be included in site-specific protocols. Chapter 6 describes the quality assurance requirements for BART analyses in the VISTAS RPO.

Recommendations

The major recommendations for VISTAS BART modeling included in this Protocol are:

I. Process

Follow the BART process steps discussed in Chapter 2:

1. Identify BART eligible sources
2. Identify which pollutants have greater than *de minimis* emission levels
3. Identify sources that are subject to BART
4. Identify baseline visibility impact of each BART source
5. Identify feasible controls and emission changes
6. Identify the change in visibility impact for each candidate BART control option
7. Compare the visibility improvement of BART control options to other statutory factors in the engineering analysis

II. CALPUFF Model Configuration

Use the CALPUFF dispersion modeling system, as described in Chapter 4, to determine if a single source is subject to BART. VISTAS will use CALPUFF Version 5.754 and CALMET Version 5.7. These versions contain enhancements funded by the Minerals Management Service (MMS) and VISTAS. They were developed by Earth Tech, Inc. and they are maintained on Earth Tech's Atmospheric Studies Group CALPUFF website (www.src.com) for public access.

VISTAS is making publicly available 12-km CALMET output files for the entire VISTAS modeling domain (eastern United States) and intends to also provide CALMET output files for five 4-km grid subdomains covering the VISTAS states and VISTAS Class I areas. To create the CALMET input files, Earth Tech used the MM5 databases developed by EPA for 2001, VISTAS for 2002, and Midwest RPO for 2003. For the 12 km grid large domain covering the entire VISTAS region, Earth Tech used the No-Obs setting (i.e., did not include additional surface and upper air observations beyond those incorporated in the MM5 calculations). For finer resolution subdomains (4 km grid or less), available surface and upper air observations will be used in addition to MM5 meteorological model outputs. The specific model settings will be provided with the CALMET files and via the CALPUFF website so that users can review or replicate the work.

For CALPUFF modeling, source emissions should be defined using the maximum 24-hour actual emission rate during normal operation for the most recent 3 or 5 years. If maximum 24-hr actual emissions are not available, continuous emissions data, permit allowable emissions, potential emissions, and emissions factors from AP-42 source profiles may be used as available.

Key points from comments received on the specific CALPUFF, CALPOST, and POSTUTIL configurations are highlighted below.

- Use CMAQ modeling data from 2001-2003 to determine background concentrations of SO_4 and total NO_3 (HNO_3 + NO_3). CMAQ data in CALPUFF-ready format will be provided for each Class I area by VISTAS. After running CALPUFF for an individual facility, repartition NO_3 in POSTUTIL using the CMAQ background data, including that for NH_3.

- Use ozone data from non-urban monitors as the background ozone input.

- Use the Pasquill-Gifford dispersion method.[1]

[1] The Final VISTAS BART Modeling Protocol (Dec. 22, 2005) recommended using turbulence-based AERMOD dispersion methods, citing EPA's *Revision to the Guideline on Air Quality Models: Adoption of a Preferred General Purpose (Flat and Complex Terrain) Dispersion Model and Other Revisions; Final Rule.* 70 FR 68218-68261. 9 November 2005. Subsequently, EPA Region IV notified the VISTAS states that using turbulence-based dispersion methods would be considered a non-guideline application of CALPUFF. Thus this Protocol has been revised to indicate Pasquill-Gifford dispersion coefficients should be used.

- In CALPOST, use Method 6 with monthly average RH for calculating extinction, as recommended by the EPA.

- Use EPA default calculations of light extinction under current and natural background conditions. In addition to the default assumptions, a source may choose to also calculate visibility using the recently revised IMPROVE algorithm described by Pitchford, et al., (2005).

Provide results in tables as illustrated in Chapter 4 that describe, for each source:

- Number of receptors within a single Class I area with impact > 0.5 dv

- Number of days at all receptors in the Class I area with impact > 0.5 dv

- Number of Class I areas with impacts > 0.5 dv

III. CALPUFF Application for BART

For determining if a BART-eligible source is subject to BART CALPUFF modeling, use a two-tier approach. For the initial exemption modeling use CALPUFF with 12-km grid CALMET. For finer resolution of meteorological fields, use CALPUFF with CALMET of 4-km or smaller grid size.

VISTAS States are accepting EPA guidance that the threshold value to establish that a source contributes to visibility impairment is 0.5 deciview.

VISTAS States are using emissions (tons per year) divided by distance (km) from a Class I area boundary (Q/d) as a presumptive indicator that a BART-eligible source is subject to BART. If Q/d for SO_2 is greater than 10 for 2002 actual annual emissions, then the State presumes that the source is subject to BART and no exemption modeling will be performed using VISTAS funds. If the source agrees with this presumption, then the source can proceed to the BART determination using CALPUFF to evaluate impacts of control options and perform the engineering analyses. If a source disagrees, the source may perform fine grid modeling to determine if its impact is <0.5 dv.

For sources with Q/d less than or equal to 10, VISTAS intends to fund Earth Tech to assist States with the initial CALPUFF exemption modeling. Each State will prioritize which sources will be offered modeling by VISTAS. Modeling of these sources will be conducted in priority order to first accommodate States with nearer term timing constraints in their SIP development process. To conserve VISTAS resources, modeling will begin with sources at lower Q/d values and continue with sources with higher Q/d values until a Q/d value that consistently results in a greater than 0.5 dv impact is identified. Chapter 4 addresses the number of VISTAS sources eligible for BART based on Q/d analysis.

Note that VISTAS does not propose to use Q/d to exempt BART-eligible sources, but only to prioritize sources for modeling purposes. Thus this application is consistent with EPA guidance not to use Q/d for exemption purposes.

For the 12-km initial modeling exemption test, compare the highest single 24-hour average value across all receptors in the Class I area to the threshold value of 0.5 dv. If the highest 24-hr average value is below 0.5 dv at all Class I areas, then the source is not subject to BART. If the highest 24-hr average value is greater than 0.5 dv, then the source may choose to perform finer grid modeling for exemption purposes or may accept determination that the source is subject to BART and proceed to establish visibility impacts prior to and after BART controls. If using the single highest 24-hr average value proves, after initial 12-km grid CALPUFF modeling, to be too conservative a screening level, VISTAS may allow some exceedances of the threshold value for exemption purposes, up to no more than the 98^{th} percentile value.

The 12-km modeling results can be used to focus finer grid modeling for exemption purposes on only those Class I areas where impacts greater than 0.5 dv were projected in the 12-km modeling.

For finer grid (4 km or less) analyses, use the 98^{th} percentile impact value for the 24-hr average. Use either the 8^{th} highest day in each year or the 22^{nd} highest day in the 3-year period, whichever is more conservative, for comparison to the exemption threshold.

Use the same model assumptions for pre-BART visibility impact and for BART control options modeling: establish baseline visibility from the pre-BART run; change one control at a time; and evaluate the change in visibility impact, i.e. the delta-deciview. Note that “no control” may constitute BART.

Visibility impact is one of the five factors considered in the engineering analysis required under the USEPA BART guideline. If a source accepts to institute the most stringent control, the engineering analyses are not required.

This common VISTAS Protocol consistently recommends conservative assumptions. Individual States ultimately have responsibility to determine which, if any, BART controls are recommended in their State Implementation Plans (SIPs).

1. INTRODUCTION AND PROTOCOL OBJECTIVES

1.1 Background

Under regional haze regulations, the Environmental Protection Agency (EPA) has issued final guidelines dated July 6, 2005 for Best Available Retrofit Technology (BART) determinations (70 FR 39104-39172). The regional haze rule includes a requirement for BART for certain large stationary sources. Sources are BART-eligible if they meet three criteria including potential emissions of at least 250 tons per year of a visibility-impairing pollutant, were put in place between August 7, 1962 and August 7, 1977, and fall within one of the 26 listed source categories in the guidance. A BART engineering evaluation using five statutory factors -- 1) existing controls; 2) cost; 3) energy and non-air environmental impacts; 4) remaining useful life of the source; 5) degree of visibility improvement expected from the application of controls -- is required for any BART-eligible source that can be reasonably expected to cause or contribute to impairment of visibility in any of the 156 federal parks and wilderness (Class I) areas protected under the regional haze rule. (Note that, depending on the five factors, the evaluation may result in no control.) Air quality modeling is an important tool available to the States to determine whether a source can be reasonably expected to contribute to visibility impairment in a Class I area.

Throughout this document the term “BART-eligible emission unit” is defined as any single emission unit that meets the criteria described above. A “BART-eligible source” is defined as the total of all BART-eligible emission units at a single facility. If a source has several emission units, only those that meet the BART-eligible criteria are included in the definition “BART-eligible source”.

One of the listed categories is steam electric plants of more than 250 million BTU/hr heat input. To determine if such a plant has greater than 250 million BTU/hr heat input and is potentially subject to BART, the boiler capacities of all electric generating units (EGUs) should be added together regardless of construction date. In this category, electric generating sources greater than 750 MW have presumptive SO_2 and NO_x emission limits. States may presume the same limits for EGU sources between 250-750 MW. However, units at those sources constructed after the BART-eligibility dates are not subject to a BART engineering evaluation. EPA, in the Clean Air Interstate Rule (CAIR), determined that an EGU participating in the CAIR trading program satisfies the BART requirements for SO_2 and NO_x. VISTAS states are tentatively accepting this guidance. CAIR does not cover PM so EGUs would still need to evaluate impacts of PM if PM emissions are above *de minimis* values.

As illustrated in Table 1-1, as of December 5, 2005, VISTAS States had identified a total of 274 BART-eligible sources that fall into 20 of the 26 BART source categories. Of the 274 sources with BART-eligible units, 84 sources are utility EGUs and 190 are non-EGU industrial sources. (Note that these numbers are not final and are subject to slight adjustments and refinements.) No BART sources are located on Tribal lands.

Table 1-1. VISTAS BART Eligible Sources

State	Total Number of Sources	EGU Sources	Non-EGU Sources
AL	48	8	40
FL	50	23	27
GA	24	10	14
KY	29	12	17
MS	18	8	10
NC	16	5	11
SC	31	6	25
TN	13	2	11
VA	18	3	15
WV	26	7	19
Total	**273**	**84**	**189**

1.2 Objective of this Protocol

The objective of this VISTAS' BART Modeling Protocol is to describe common procedures for air quality modeling to support BART determinations that are consistent with the EPA guidelines. The protocol will serve as the basis for establishing a common understanding among the organizations who will be performing the BART analyses or reviewing the BART modeling results, including VISTAS State and Local air regulatory agencies, EPA, Federal Land Managers (FLMs), source operators, and contractors for the sources. This final protocol incorporates EPA final guidance and comments that were received on VISTAS' draft protocol[2] and provides additional description of modeling procedures.

The VISTAS States have accepted EPA's guidance to use the CALPUFF modeling system to comply with the BART modeling requirements of the regional haze rule. A BART-eligible source will be required to submit a site-specific modeling protocol to the State for review and approval prior to performing CALPUFF modeling. States will consult with FLMs and the EPA when evaluating the site-specific BART protocols. The site-specific protocol will include the source-specific data on source location, stack parameters, and emissions. The methods of the

[2] *Draft Protocol for the Application of the CALPUFF Model for Analyses of Best Available Retrofit Technology (BART). VISTAS*, March 22, 2005 and September 20, 2005.

VISTAS common modeling protocol will be followed in the site-specific protocol unless the source proposes to the State, and the State approves, alternative methods or assumptions.

Each VISTAS State or Local agency retains responsibility for the specific procedures and processes it will follow in working with the BART sources under its jurisdiction, the FLMs, EPA, and public to determine BART controls for sources in the State. Nothing in the VISTAS process replaces States' responsibility to determine BART controls.

The remainder of this document describes the CALPUFF modeling system and the application of CALPUFF to two situations:

- Air quality modeling to determine whether a BART-eligible source is "subject to BART" and therefore the BART analysis process must be applied to its operations.
- Air quality modeling of emissions from sources that have been found to be subject to BART, to evaluate regional haze benefits of alternative control options and to document the benefits of the preferred option.

Chapters 2 and 3 of this document are intended to provide background information on EPA's guidance for BART analysis modeling and on the CALPUFF modeling system. Subsequent chapters include more specific recommendations. Chapter 2 of this document reviews EPA's guidance for regional haze BART analysis modeling, as outlined in the 6 July 2005 Federal Register notice. The CALPUFF model is the preferred model recommended by the EPA for BART modeling analyses and its characteristics and limitations are discussed in Chapter 3. The specific steps to determine whether a BART-eligible source is subject to BART and to evaluate BART controls are described in Chapter 4. The procedures include initial modeling of BART-eligible sources using CALPUFF run in a conservative mode with regional meteorological datasets. For sources determined to be subject to BART based on these first modeling analyses, further finer grid CALPUFF analyses would be performed. The model configuration for the common modeling protocol is described in Chapter 4. Details of the source-specific protocol are described in Chapter 5. A quality assurance plan is outlined in Chapter 6.

EPA's guidance allows for the use of appropriate alternative models, however VISTAS will not develop a protocol for alternative models. This protocol focuses on guidance for the application of the preferred CALPUFF modeling approach. If a source wants to use an alternative model in its BART demonstration, the source will need to submit a detailed written justification to the State for review and approval. The State will provide the documentation to the EPA and Federal Land Managers for their review.

Also, this protocol does not address a preferred modeling approach to demonstrate the effectiveness of an optional emissions cap and trade program. Such a cap and trade program is not required, but can be implemented in lieu of BART if desired by the VISTAS States. VISTAS States are not pursuing a regional trading alternative under the proposed EPA trading guidance (70 FR 44154-44175) that is to be promulgated early in 2006.

2. REVIEW OF EPA'S GUIDANCE FOR BART MODELING

The final guidance for regional haze BART determinations was published in the Federal Register on 6 July 2005 (70 FR 39104 to 39172). It prescribes the modeling approaches that are to be used for various stages of the BART analysis process.

This chapter provides a summary of EPA's guidance for BART modeling. It is not intended to provide a comprehensive review of the guidance. Nor does this chapter address specific recommendations for VISTAS' approach to CALPUFF BART modeling. Those recommendations appear in Chapter 4.

2.1 Overview of the Regional Haze BART Process

The process of establishing BART emission limitations consists of four steps:

1) Identify whether a source is "BART-eligible" based on its source category, when it was put in service, and the magnitude of its emissions of one or more "visibility-impairing" air pollutants. The BART guidelines list 26 source categories of stationary sources that are BART-eligible. Sources must have been put in service between August 7, 1962 and August 7, 1977 in order to be BART-eligible. Finally, a source is eligible for BART if potential emissions of visibility-impairing air pollutants are greater than 250 tons per year. Qualifying pollutants include primary particulate matter (PM_{10}) and gaseous precursors to secondary fine particulate matter, such as SO_2 and NO_x. Whether ammonia or volatile organic compounds (VOCs) should be included as visibility-impairing pollutants for BART eligibility is left for the States to determine on a case-by-case basis. The guidance states that high molecular weight VOCs with 25 or more carbon atoms and low vapor pressure should be considered as primary $PM_{2.5}$ emissions and not VOCs for BART purposes.

(Note: If the source is subject to BART because one visibility impairing pollutant has potential emissions > 250 TPY, the State may determine that other visibility impairing pollutants are not subject to BART if their potential emissions are less than the *de minimis* levels (40 TPY for SO_2 and NO_x and 15 TPY of PM_{10} or $PM_{2.5}$. This assumes that the other BART-eligibility criteria are met.)

2) Determine whether a BART-eligible source can be excluded from BART controls by demonstrating that the source cannot be reasonably expected to cause or contribute to visibility impairment in a Class I area. The preferred approach is an assessment with an air quality model such as CALPUFF or other appropriate model followed by comparison of the estimated 24-hr visibility impacts against a threshold above estimated natural conditions to be determined by the States.[3] The threshold to determine whether a single source "causes" visibility impairment is set at

[3] The level of the natural conditions baseline that is to be used is described differently in the BART guideline and in the preamble to the BART rule. The BART guideline text says "natural conditions" at 70 FR 39162, col. 3, while the preamble says "natural visibility baseline for the 20% best visibility days" at 70 FR 39125, col. 1. Clarification received from Todd Hawes, US EPA, is that the intent was the 20% best days.

1.0 deciview change from natural conditions over a 24-hour averaging period in the final BART rule (70 FR 39118). The guidance also states that the proposed threshold at which a source may "contribute" to visibility impairment should not be higher than 0.5 deciviews although, depending on factors affecting a specific Class I area, it may be set lower than 0.5 deciviews. The test against the threshold is "driven" by the contribution level, since if a source "causes", by definition it "contributes".

EPA recommends that the 98th percentile value from the modeling be compared to the contribution threshold of 0.5 deciviews (or a lower level set by a State) to determine if a source does not contribute to visibility impairment and therefore is not subject to BART. Whether or not the 98th percentile value exceeds the threshold must be determined at each Class I area. Over an annual period, this implies the 8th highest 24-hr value at a particular Class I area is compared to the contribution threshold. Over a 3-year modeling period, the 98th percentile value may be interpreted as the highest of the three annual 98th percentile values at a particular Class I area or the 22nd highest value in the combined three year record, whichever is more conservative.

Alternatively, States have the option of considering that all BART-eligible sources within the State are subject to BART and skipping the initial impact analysis. In rare cases, a State might be able to do exactly the opposite, and use regional modeling to conclude that all BART-eligible sources in the State do not cumulatively contribute to "measurable" visibility impairment in any Class I areas. Also, the States have an option to exempt individual sources based on model plant analysis conducted by EPA in finalizing the BART rule. Under this option, sources with potential emissions of SO_2 plus NO_x of less than 500 tons and a distance from any Class I area greater than 50 kilometers or sources with SO_2 plus NO_x potential emissions of less than 1000 tons and a distance from any Class I area greater than 100 kilometers can be exempted. PM emissions are not specifically addressed in the model plant analysis, but subsequent discussions with EPA staff indicate that PM may be considered along with SO_2 and NO_x, so that a plant could be exempted if the combined potential emissions of SO_2, NO_x, plus PM meet the criteria above.

3) Determine BART controls for the source by considering various control options and selecting the "best" alternative, taking into consideration:

a) Any pollution control equipment in use at the source (which affects the availability of options and their impacts),

b) The costs of compliance with control options,

c) The remaining useful life of the facility,

d) The energy and non air-quality environmental impacts of compliance, and

e) The degree of improvement in visibility that may reasonably be anticipated to result from the use of such technology.

Note that if a source agrees to apply the most stringent controls available to BART-eligible units, the BART analysis is essentially complete and no further analysis is necessary (70 FR 39165).

4) Incorporate the BART determination into the State Implementation Plan for Regional Haze, which is due by December 2007.

Instead of applying BART on a source-by-source basis, a State (or a group of States) has the option of implementing an emissions trading program that is designed to achieve regional haze improvements that are greater than the visibility improvements that could be expected from BART. If the geographic distributions of emissions under the two approaches are similar, determining whether trading is "better than BART" may be possible by simply comparing emissions expected under the trading program against the emissions that could be expected if BART was applied to eligible sources. If the geographic distributions of emissions are likely to be different, however, air quality modeling comparing the expected improvements in visibility from the trading program and from BART would be required. (See the proposed BART Alternative rule, at 70 FR 44160.) EPA suggests that regional modeling using a photochemical grid model may be more appropriate than CALPUFF for this purpose.

Note that EPA has indicated in the BART rule (70 FR 39138-39139) that emissions reductions under the Clean Air Interstate Rule (CAIR) meet the BART requirement for SO_2 and NO_x control for those EGUs subject to BART. However, PM emissions from EGUs are not addressed by CAIR and therefore a BART analysis may still be required for PM.

2.2 Model Recommendations for the BART Analysis

To evaluate the visibility impacts of a BART-eligible source at Class I areas beyond 50 km from the source, the EPA guidance recommends the use of the CALPUFF model as "the best regulatory modeling application currently available for predicting a single source's contribution to visibility impairment" (70 FR 39162). The use of another "appropriate model" is allowed although the EPA prefers the use of CALPUFF. If a source wants to use an alternative model, the source needs to submit a written justification and source-specific modeling protocol to its State for review and approval. As part of the consultation process, the State will provide documentation to EPA and FLM.

For modeling the impact of a source closer than 50 km to a Class I area, EPA's BART guidance recommends that expert modeling judgment be used, "giving consideration to both CALPUFF and other methods." The PLUVUE-II plume visibility model is mentioned as a possible model to consider instead of CALPUFF for a source within less than 50 km of a Class I area**.**

The EPA guidance notes that "regional scale photochemical grid models may have merit, but such models have been designed to assess cumulative impacts, not impacts from individual sources" and they are "very resource intensive and time consuming relative to CALPUFF", but States may consider their use for SIP development in the future as they may be adapted and "demonstrated to be appropriate for single source applications" (70 FR 39123). Photochemical grid models may be more appropriate for cumulative modeling options such as in the determination of the aggregate contribution of all-BART-eligible sources to visibility impairment, but such use should involve consultation with the appropriate EPA Regional Office (70 FR 39163).

According to the BART guidance, a modeling protocol should be submitted for all modeling demonstrations regardless of the distance from the BART-eligible source to the Class I area. EPA's role in the development of the protocol is only advisory as the "States better understand the BART-eligible source configurations" and factors affecting their particular Class I areas (70 FR 39126).

In the BART modeling analyses the EPA recommends that the State use the highest 24-hour average actual emission rate for the most recent three to five-year period of record. Emissions on days influenced by periods of start-up, shutdown and malfunction are not to be considered in determining the appropriate emission rates. (70 FR 39129).

If a source is found to be subject to BART, CALPUFF or another appropriate model should be used to evaluate the improvement in visibility resulting from the application of BART controls. Visibility improvements may be evaluated on a pollutant-specific basis in the BART determination (70 FR 39129).

For evaluating the improvement in visibility resulting from the application of BART, the EPA guidelines state that States are "encouraged to account for the magnitude, frequency, and duration of the contributions to visibility impairment caused by the source based on the natural variability of meteorology" (70 FR 39129).

2.3 Performance of a Cap and Trade Program

If a State or States elect to pursue an optional cap and trade program, they are required to demonstrate greater "reasonable progress" in reducing haze than would result if BART were applied to the same sources. In some cases, a State may simply be able to demonstrate that a trading program that achieves greater progress at reducing emissions will also achieve greater progress at reducing haze. Such would be the case if the likely geographic distribution of emissions under the trading program would not be greatly different from the distribution if BART was in place.

If the expected distribution of emissions is different under the two approaches, then "dispersion modeling" of all sources must be used to determine the difference in visibility at each impacted Class I area, in order to establish that the optional trading program will result in visibility improvements aggregated over all Class I areas that are "better than BART" (70 FR 39137-39138). The BART guidance does not specify the method to be used for this modeling. From a technical perspective, either applying CALPUFF to every source or using a regional photochemical model would satisfy the need.

A rulemaking procedure is currently underway to establish final guidance for such alternatives to BART (70 FR 44154-44175). The rule is expected to be finalized early in 2006.

3. OVERVIEW OF THE CALPUFF MODELING SYSTEM

This chapter contains a general description of the CALPUFF modeling system and its capabilities and limitations. It does not include specific recommendations regarding the use of the model for BART analysis in the VISTAS region. These specific recommendations can be found in Chapter 4.

3.1 Capabilities and features of CALPUFF

The CALPUFF modeling system (Scire et al., 2000a, b) is recommended as the preferred modeling approach for use in the BART analyses. CALPUFF and its meteorological model, CALMET, are designed to handle the complexities posed by the complex terrain, the large source-receptor distances, chemical transformation and deposition, and other issues related to Class I visibility impacts. The CALPUFF modeling system has been adopted by the EPA as a *Guideline Model* for source-receptor distances greater than 50 km, and for use on a case-by-case basis in complex flow situations for shorter distances (68 FR 18440-18482). CALPUFF is recommended for Class I impact assessments by the Federal Land Managers Workgroup (FLAG 2000) and the Interagency Workgroup on Air Quality Modeling (IWAQM) (EPA 1998). The final BART guidance recommends CALPUFF as “the best modeling application available for predicting a singe source’s contribution to visibility impairment” (70 FR 39122). As a result of these recommendations, the VISTAS modeling protocol is based on the use of CALPUFF for its BART determinations.

The main components of the CALPUFF modeling system are shown in Figure 3-1. CALMET is a diagnostic meteorological model that is used to drive the CALPUFF dispersion model. It produces three-dimensional wind and temperature fields and two-dimensional fields of mixing heights and other meteorological fields. It contains slope flow effects, terrain channeling, and kinematic effects of terrain. CALMET includes special algorithms for treating the overwater boundary layer and coastal interaction effects. CALMET can use meteorological observational data and/or three-dimensional output from prognostic numerical meteorological models such as MM5 (Grell et al., 1995) or RUC (Benjamin et al., 2004) in the developments of its fine-scale meteorological fields.

CALPUFF is a non-steady-state Lagrangian puff transport and dispersion model that advects Gaussian puffs of multiple pollutants from modeled sources. CALPUFF’s algorithms have been designed to be applicable on spatial scales from a few tens of meters to hundreds of kilometers from a source. It includes algorithms for near-field effects such as building downwash, stack tip downwash and transitional plume rise as well as processes important in the far-field such as chemical transformation, wet deposition, and dry deposition. CALPUFF contains an option to allow puff splitting in the horizontal and vertical directions, which extends the distance range of the model. The primary outputs from CALPUFF are hourly concentrations and hourly deposition fluxes evaluated at user-specified receptor locations.

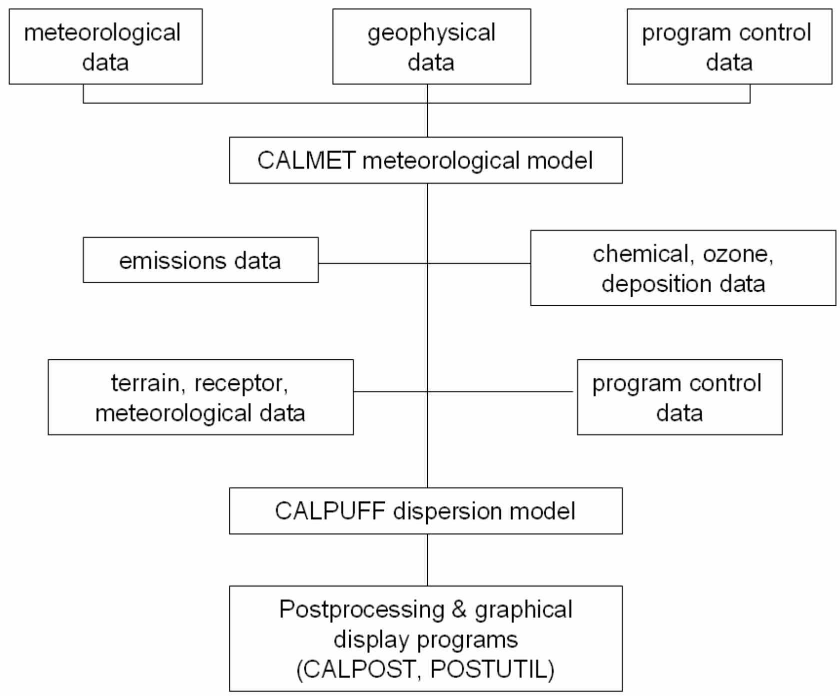

Figure 3-1. CALPUFF modeling system components.

A set of postprocessing programs associated with CALPUFF computes visibility effects and allows cumulative source impacts to be assessed, including potential non-linear effects of ammonia limitation on nitrate formation. The CALPOST postprocessor contains several options for computing change in extinction and deciviews for visibility assessments. The POSTUTIL postprocessor includes options for summing contributions of individual sources or groups of sources to assess cumulative impacts. POSTUTIL also contains CALPUFF's nitric acid-nitrate chemical equilibrium module, which allows the cumulative effects of ammonia consumption by background sources to be assessed in the postprocessor. In addition, the combination of CALPUFF and POSTUTIL allows the effects of source emissions of ammonia to be incrementally added to background ammonia levels when determining nitrate formation.

The rest of this chapter summarizes the capabilities and features of the CALPUFF modeling components in more detail.

3.1.1 Major Features of CALMET

The CALMET meteorological model consists of a diagnostic wind field module and micrometeorological modules for overwater and overland boundary layers. When modeling a large geographical area, as would be necessary for the regional VISTAS domain, the user has the option to use a Lambert Conformal Projection coordinate system to account for Earth's curvature.

The major features and options of the meteorological model are summarized in Table 3-1. The techniques used in the CALMET model are briefly described below.

Table 3-1. Major Features of the CALMET Meteorological Model

- **Boundary Layer Modules of CALMET**
  - Overland Boundary Layer - Energy Balance Method
  - Overwater Boundary Layer - Profile Method
    - -- COARE algorithm
    - -- OCD-based method
  - Produces Gridded Fields of:
    - -- Surface Friction Velocity
    - -- Convective Velocity Scale
    - -- Monin-Obukhov Length
    - -- Mixing Height
    - -- PGT Stability Class
    - -- Air Temperature (3-D)
    - -- Precipitation Rate

- **Diagnostic Wind Field Module of CALMET**
  - Slope Flows
  - Kinematic Terrain Effects
  - Terrain Blocking Effects
  - Divergence Minimization
  - Produces Gridded Fields of U, V, W Wind Components
  - Inputs Include Domain-Scale Winds, Observations, and (optionally) Coarse-Grid Prognostic Model Winds
  - Lambert Conformal Projection Capability

CALMET Boundary Layer Models

The CALMET model contains two boundary layer models for application to overland and overwater grid cells.

Overland Boundary Layer Model: Over land surfaces, the energy balance method of Holtslag and van Ulden (1983) is used to compute hourly gridded fields of the sensible heat flux, surface friction velocity, Monin-Obukhov length, and convective velocity scale. Mixing heights are determined from the computed hourly surface heat fluxes and observed temperature soundings using a modified Carson (1973) method based on Maul (1980). The model also determines gridded fields of Pasquill-Gifford-Turner (PGT) stability class and hourly precipitation rates.

Overwater Boundary Layer Model: The aerodynamic and thermal properties of water surfaces suggest that a different method is best suited for calculating the boundary layer parameters in the marine environment. A profile technique, using air-sea temperature differences, is used in CALMET to compute the micro-meteorological parameters in the marine boundary layer. The version of CALMET being used by VISTAS contains improvements in the overwater boundary layer parameterizations (Fairall et al., 2003) based on the Coupled Ocean Atmosphere Response Experiment (COARE) and enhancements in the calculation of overwater mixed layer heights (Batchvarova and Gryning, 1991, 1994). Further details and the results of an evaluation of the model containing these enhancements are described in Scire et al. (2005). An upwind-looking spatial averaging scheme is optionally applied to the mixing heights and three-dimensional temperature fields in order to account for important advective effects.

Diagnostic Wind Field Module

The diagnostic wind field module uses a two-step approach to the computation of the wind fields (Douglas and Kessler, 1988). In the first step, an initial-guess wind field is adjusted for kinematic effects of terrain, slope flows, and terrain blocking effects to produce a Step 1 wind field. Gridded MM5 can be used to define the initial guess field. The second step consists of an objective analysis procedure to introduce observational data into the Step 1 wind field to produce a final wind field.

Step 1 Wind Field. Development of the Step 1 wind field begins with the initial guess field defined by the MM5 prognostic meteorological model. Normally, the CALMET computational domain is specified to be at finer grid resolution than the MM5 dataset used to initialize the initial guess field. For example, 36-km MM5 data available for VISTAS modeling may be used to develop the initial guess field on a 12-km or even a 1-km CALMET grid. The Step 1 algorithms in CALMET described below apply terrain adjustments to the initial guess field on the fine-scale CALMET grid. Thus, the CALMET winds are adjusted to respond to fine-scale terrain features not necessarily seen by the coarser scale MM5 model.

Kinematic Effects of Terrain: The approach of Liu and Yocke (1980) is used to evaluate the effects of the terrain on the wind field. The initial guess field winds are used to compute a terrain-forced vertical velocity, subject to an exponential, stability-dependent decay function. The effects of terrain on the horizontal wind components are evaluated by applying a divergence-minimization scheme to the initial guess wind field. The divergence minimization scheme is applied iteratively until the three-dimensional divergence is less than a threshold value.

Slope Flows: The original slope flow algorithm in CALMET has been upgraded (Scire and Robe, 1997) based on the shooting flow algorithm of Mahrt (1982). This scheme includes both advective-gravity and equilibrium flow regimes. At night, the slope flow model parameterizes the flow down the sides of the valley walls into the floor of the valley, and during the day, upslope flows are parameterized. The magnitude of the slope flow depends on the local surface sensible heat flux and local terrain gradients. The slope flow wind components are added to the wind field adjusted for kinematic effects.

Blocking Effects: The thermodynamic blocking effects of terrain on the wind flow are parameterized in terms of the local Froude number (Allwine and Whiteman, 1985). If the Froude number at a particular grid point is less than a critical value and the wind has an uphill component, the wind direction is adjusted to be tangent to the terrain.

Step 2 Wind Field. The wind field resulting from the above adjustments of the initial-guess wind is the Step 1 wind field. The second step of the procedure may involve introduction of observational data into the Step 1 wind field through an objective analysis procedure. An inverse-distance squared interpolation scheme is used which weights observational data heavily in the vicinity of the observational station, while the Step 1 wind field dominates the interpolated wind field in regions with no observational data. The resulting wind field is subject to smoothing, an optional adjustment of vertical velocities based on the O'Brien (1970) method, and divergence minimization to produce a final Step 2 wind field.

The introduction of observational data in the Step 2 calculation is an option. It is also possible to run the model in "no observations" (No-Obs) mode, which involves the use only of MM5 gridded data for the initial guess field followed by fine-scale terrain adjustments by CALMET. In No-Obs mode, observational data are not used in the Step 2 calculations. The No-Obs mode is appropriate when the MM5 simulations adequately characterize the regional wind patterns and when local observations, especially surface observations, reflect local conditions on a scale smaller than that of the CALMET domain and hence their spatial representativeness may be limited. Such situations are most likely to occur when the CALMET grid scale is relatively large i.e., coarser than the scale of variation of the true wind field, which is particularly likely to occur in complex terrain or along the seashore,

3.1.2 Major Features of CALPUFF

By its puff-based formulation and through the use of three-dimensional meteorological data developed by the CALMET meteorological model, CALPUFF can simulate the effects of time- and space-varying meteorological conditions on pollutant transport from sources in complex terrain. The major features and options of the CALPUFF model are summarized in Table 3-2. Some of the technical algorithms are briefly described below.

Complex Terrain: The effects of complex terrain on puff transport are derived from the CALMET winds. In addition, puff-terrain interactions at gridded and discrete receptor locations are simulated using one of two algorithms that modify the puff-height (either that of ISCST3 or a general "plume path coefficient" adjustment), or an algorithm that simulates enhanced vertical dispersion derived from the weakly-stratified flow and dispersion module of the Complex Terrain

Dispersion Model (CTDMPLUS) (Perry et al., 1989). The puff-height adjustment algorithms rely on the receptor elevation (relative to the elevation at the source) and the height of the puff above the surface. The enhanced dispersion adjustment relies on the slope of the gridded terrain in the direction of transport during the time step.

Subgrid Scale Complex Terrain (CTSG): An optional module in CALPUFF, CTSG treats terrain features that are not resolved by the gridded terrain field, and is based on the CTDMPLUS (Perry et al., 1989). Plume impingement on subgrid-scale hills is evaluated at the CTSG subgroup of receptors using a dividing streamline height (H_d) to determine which pollutant material is deflected around the sides of a hill (below H_d) and which material is advected over the hill (above H_d). The local flow (near the feature) used to define H_d is taken from the gridded CALMET fields. As in CTDMPLUS, each feature is modeled in isolation with its own set of receptors.

Puff Sampling Functions: A set of accurate and computationally efficient puff sampling routines is included in CALPUFF, which solve many of the computational difficulties encountered when applying a puff model to near-field releases. For near-field applications during rapidly-varying meteorological conditions, an elongated puff (slug) sampling function may be used. An integrated puff approach may be used during less demanding conditions. Both techniques reproduce continuous plume results under the appropriate steady state conditions.

Building Downwash: The Huber-Snyder and Schulman-Scire downwash models are both incorporated into CALPUFF. An option is provided to use either model for all stacks, or make the choice on a stack-by-stack and wind sector-by-wind sector basis. Both algorithms have been implemented in such a way as to allow the use of wind direction specific building dimensions. The PRIME building downwash model (Schulman et al., 2000) is also included in CALPUFF as an option.

Dispersion Coefficients: Several options are provided in CALPUFF for the computation of dispersion coefficients, including the use of turbulence measurements (σ_v and σ_w), the use of similarity theory to estimate σ_v and σ_w from modeled surface heat and momentum fluxes, or the use of Pasquill-Gifford (PG) or McElroy-Pooler (MP) dispersion coefficients, or dispersion equations based on the CTDM. Options are provided to apply an averaging time correction or surface roughness length adjustments to the PG coefficients. In version 5.754 of CALPUFF being used by VISTAS, an option is provided to use the AERMOD turbulence profiles for determining dispersion rates, which is the most recent approach to dispersion in EPA-approved regulatory modeling. In addition, turbulence advection is included. For additional details on these features, see Scire et al. (2005).

Overwater and Coastal Interaction Effects: Because the CALMET meteorological model contains both overwater and overland boundary layer algorithms, the effects of water bodies on plume transport, dispersion, and deposition can be simulated with CALPUFF. The puff formulation of CALPUFF is designed to handle spatial changes in meteorological and dispersion conditions, including the abrupt changes that occur at the coastline of a major body of water.

Dry Deposition: A resistance model is provided in CALPUFF for the computation of dry deposition rates of gases and particulate matter as a function of geophysical parameters, meteorological conditions, and pollutant species. For particles, source-specific mass distributions may be provided for use in the resistance model. Of particular interest for BART analyses is the ability to separately model the deposition of fine particulate matter (< 2.5 μm diameter) from coarse particulate matter (2.5-10 μm diameter).

Wind Shear Effects: CALPUFF contains an optional puff splitting algorithm that allows vertical wind shear effects across individual puffs to be simulated. Differential rates of dispersion and transport among the "new" puffs generated from the original, well-mixed puff can substantially increase the effective rate of horizontal spread of the material. Puffs may also be split in the horizontal when the puff size becomes large relative to the grid size, to account for wind shear across the puffs.

Wet Deposition: An empirical scavenging coefficient approach is used in CALPUFF to compute the depletion and wet deposition fluxes due to precipitation scavenging. The scavenging coefficients are specified as a function of the pollutant and precipitation type (i.e., frozen vs. liquid precipitation).

Chemical Transformation: CALPUFF includes options for parameterizing chemical transformation effects using the five species scheme (SO_2, $SO_4^{=}$, NO_x, HNO_3, and NO_3^-) employed in the MESOPUFF II model or a set of user-specified, diurnally-varying transformation rates. The MESOPUFF II scheme is recommended by IWAQM. It produces secondary fine particulate matter (sulfate and nitrate) from emissions of SO_2 and NO_x and thus allows analyses of visibility impacts. Ambient ozone concentrations are used in the parameterized chemical transformation module as a surrogate for OH radicals during daylight hours. Ambient ammonia concentrations are used together with a temperature and relative humidity-dependent equilibrium relationship to partition nitric acid and nitrate on an hour-by-hour and receptor-by-receptor basis.

Table 3-2. Major Features of the CALPUFF Dispersion Model

- **Source types**
  - Point sources (constant or variable emissions)
  - Line sources (constant or variable emissions)
  - Volume sources (constant or variable emissions)
  - Area sources (constant or variable emissions)

- **Non-steady-state emissions and meteorological conditions**
  - Gridded 3-D fields of meteorological variables (winds, temperature)
  - Spatially-variable fields of mixing height, friction velocity, convective velocity scale, Monin-Obukhov length, precipitation rate
  - Vertically and horizontally-varying turbulence and dispersion rates
  - Time-dependent source and emissions data for point, area, and volume sources
  - Temporal or wind-dependent scaling factors for emission rates, for all source types

- **Interface to the Emissions Production Model (EPM)**
  - Time-varying heat flux and emissions from controlled burns and wildfires

- **Efficient sampling functions**
  - Integrated puff formulation
  - Elongated puff (slug) formulation

- **Dispersion coefficient (σ_y, σ_z) options**
  - Direct measurements of σ_v and σ_w
  - Estimated values of σ_v and σ_w based on similarity theory
    - -- AERMOD turbulence profiles
    - -- Original turbulence profiles
  - Pasquill-Gifford (PG) dispersion coefficients (rural areas)
  - McElroy-Pooler (MP) dispersion coefficients (urban areas)
  - CTDM dispersion coefficients (neutral/stable)

- **Vertical wind shear**
  - Puff splitting
  - Differential advection and dispersion

- **Plume rise**
  - Buoyant and momentum rise
  - Stack tip effects
  - Building downwash effects
  - Partial penetration
  - Vertical wind shear

- **Building downwash**
  - Huber-Snyder method
  - Schulman-Scire method
  - PRIME method

- **Complex terrain**
  - Steering effects in CALMET wind field
  - Optional puff height adjustment: ISC3 or "plume path coefficient"
  - Optional enhanced vertical dispersion (neutral/weakly stable flow in CTDMPLUS)

Table 3-2. Major Features of the CALPUFF Dispersion Model (Cont'd)

- **Subgrid scale complex terrain (CTSG option)**
  - Dividing streamline, H_d, as in CTDMPLUS:
    - Above H_d, material flows over the hill and experiences altered diffusion rates
    - Below H_d, material deflects around the hill, splits, and wraps around the hill

- **Dry Deposition**
  - Gases and particulate matter
  - Three options:
    - Full treatment of space and time variations of deposition with a resistance model
    - User-specified diurnal cycles for each pollutant
    - No dry deposition

- **Overwater and coastal interaction effects**
  - Overwater boundary layer parameters (COARE algorithm or OCD-based method)
  - Abrupt change in meteorological conditions, plume dispersion at coastal boundary
  - Plume fumigation

- **Chemical transformation options**
  - Pseudo-first-order chemical mechanism for SO_2, $SO_4^{=}$, NO_x, HNO_3, and NO_3^- (MESOPUFF II method)
  - Pseudo-first-order chemical mechanism for SO_2, $SO_4^{=}$, NO, NO_2, HNO_3, and NO_3^- (RIVAD/ARM3 method)
  - User-specified diurnal cycles of transformation rates
  - No chemical conversion

- **Wet Removal**
  - Scavenging coefficient approach
  - Removal rate a function of precipitation intensity and precipitation type

3.1.3 Major Features of Postprocessors (CALPOST and POSTUTIL)

The two main postprocessors of interest for BART applications are the CALPOST and POSTUTIL programs. CALPOST is used to process the CALPUFF outputs, producing tabulations that summarize the results of the simulations, identifying, for example, the highest and second-highest hourly-average concentrations at each receptor. When performing visibility-related modeling, CALPOST uses concentrations from CALPUFF to compute light extinction and related measures of visibility (haze index in deciviews), reporting these for a 24-hour averaging time.

The CALPOST processor contains several options for evaluating visibility impacts, including the method described in the BART guidance, which uses monthly average relative humidity values. CALPOST contains implementations of the IWAQM-recommended and FLAG-recommended visibility techniques and additional options to evaluate the impact of natural weather events (fog, rain and snow) on background visibility and visibility impacts from modeled sources.

The POSTUTIL processor is a program that allows the cumulative impacts of multiple sources from different simulations to be summed, can compute the difference between two sets of predicted impacts (useful for evaluating the benefits of BART controls), and contains a chemistry module to evaluate the equilibrium relationship between nitric acid and nitrate aerosols. This capability allows the potential non-linear effects of ammonia scavenging by sulfate and nitrate sources to be evaluated in the formation of nitrate from an individual source. CALPUFF makes the full ambient ammonia concentration available to each puff without regard for any scavenging by other puffs. POSTUTIL corrects for such scavenging when the puffs generated by the CALPUFF model overlap, as could be the case for a single source when the wind speed is low, or when nitrate formation is to be attributed to each of several sources that are in a cluster and whose plumes overlap,

POSTUTIL will also compute the impacts of individual sources or groups of sources on sulfur and nitrogen deposition into aquatic, forest and coastal ecosystems. The postprocessor allows the changes in deposition fluxes resulting from changes in emissions to be quantified. For example the output of POSTUTIL and CALPOST can be used as input into an Acid Neutralizing Capacity (ANC) analysis, or for comparison to Deposition Analysis Thresholds (DATs).

3.2 Discussion of CALPUFF Applicability and Limitations

3.2.1 Transport and Diffusion

According to the IWAQM Phase 2 report (page 18), "CALPUFF is recommended for transport distances of 200 km or less. Use of CALPUFF for characterizing transport beyond 200 to 300 km should be done cautiously with an awareness of the likely problems involved."[4]

IWAQM's 200-km limitation derives from the observation that, when compared to the data of the Cross Appalachian Tracer Experiment (CAPTEX), the basic configuration of CALPUFF overestimated inert tracer concentrations by factors of 3 to 4 at receptors that were 300 to 1000 km from the source. The apparent reason was insufficient horizontal dispersion of the simulated plume, presumably because an actual large plume does not remain coherent in the presence of vertical wind shears that typically occur, especially during the night, and of horizontal wind shears over the large puffs that arise over long transport distances.

To better represent such situations, an optional puff splitting algorithm has since been added to CALPUFF to simulate wind shear effects across a well-mixed individual puff by dividing the puff horizontally and vertically into two or more pieces. Differential rates of transport among the

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[4] The IWAQM presentation at EPA's 6th Modeling Conference provides the background for this recommendation: "The IWAQM concludes that CALPUFF be recommended as providing unbiased estimates of concentration impacts for transport distances of order 200 km and less, and for transport times of order 12 hours or less. For larger transport times and distances, our experience thus far is that CALPUFF tends to underestimate the horizontal extent of the dispersion and hence tends to overestimate the surface-level concentration maxima. This does not preclude the use of CALPUFF for transport beyond 300 km, but it does suggest that results in such instances be used cautiously and with some understanding." (From page D-12 of the IWAQM Phase 2 report.)

new puffs thus generated can increase the horizontal spread of the material in the plume due to vertical wind speed shear and wind direction shear. The horizontal puff splitting algorithm is designed to allow large puffs that may grow to be several grid cells or more in size to split into smaller puffs that can then more accurately respond to variations in the local wind field across the original large puff. This will also tend to increase horizontal dispersion of the plume. Since the creation of additional puffs via puff splitting will increase the computational requirements of the model, possibly substantially, puff splitting is not enabled by default, but can be turned on at the option of the user. Puff splitting may be appropriate for transport distances over 200 to 300 km, or possibly over shorter distances in complex terrain.

Turning to the shorter distance end of the transport range, the CALPUFF section of Appendix A of the *Guideline on Air Quality Models* (40 CFR 51, Appendix W) states, "CALPUFF is intended for use on scales from tens of meters from a source to hundreds of kilometers." This is supported by the IWAQM Phase 2 report, which indicates that the diffusion algorithms in CALPUFF were designed to be suitable for both short and long distances. In this regard, CALPUFF does contain algorithms for such near-field effects as plume rise, building downwash, and terrain impingement and includes routines that deal with the computational difficulties encountered when applying a puff model in the field near to a source.

The recommendations for regulatory use in Appendix A of the *Guideline on Air Quality Models* state, "CALPUFF is appropriate for long range transport (source-receptor distance of 50 to several hundred kilometers)", but provisions for using CALPUFF in the near-field in "complex flow" situations are also included in the regulatory guidance. Complex flow situations may include complex terrain, coastal areas, situations where plume fumigation is likely, and areas where stagnation, flow reversals, recirculation or spatial variability in wind fields (e.g., as due to changes in valley orientation) are important.

The tracer studies with which CALPUFF transport and diffusion capabilities were evaluated in the IWAQM Phase 2 report were generally over distances greater than 50 km. More recently, additional studies of model performance have been performed at shorter distances, including at a power plant in New York state in complex terrain (at source-receptor distances of 2 to 8.5 km) and a second power plant in Illinois in simple terrain (at source-receptor distances in arcs ranging from 0.5 km to 50 km from the stack) (Strimaitis et al., 1998). Other CALPUFF evaluation studies over short-distances include ones by Chang et al. (2001) and Morrison et al. (2003). These studies demonstrate good model performance over source-receptor distances from a few hundred meters to 50 km.

An important factor in the performance of CALPUFF is the choice of dispersion coefficients. The EPA has defined the "regulatory default" option in CALPUFF to allow either Pasquill-Gifford (PG) or turbulence-based dispersion coefficients. CALPUFF has been evaluated and shown to perform better using turbulence-based dispersion for tall stacks (Strimaitis et al, 1998). CALPUFF with turbulence-based dispersion has also been evaluated for overwater transport and coastal situations (Scire et al., 2005). In many other studies, including AERMOD evaluation studies conducted by EPA, the use of PG-dispersion, or more specifically the lack of a convective probability density function (pdf) module, has been demonstrated to result in underprediction of peak concentrations.

In November 2005, EPA approved the AERMOD model, which relies on turbulence-based dispersion, as a regulatory Guideline Model[5]. The ISCST3 model and its PG dispersion coefficients are being phased out as an acceptable regulatory approach. However, EPA Region IV has indicated that the application of turbulence-based dispersion coefficients in CALPUFF needs to be further demonstrated before they are approved for BART application. They will consider accepting the use of turbulence dispersion coefficients on a case-by-case basis for sources that are close to Class I areas.

For regional haze light extinction calculations, use of a plume-simulating model such as CALPUFF is appropriate only when the plume is sufficiently diffuse that it is not visually discernible as a plume *per se*, but nevertheless its presence could alter the visibility through the background haze. The IWAQM Phase 2 report states that such conditions occur starting 30 to 50 km from a source. In this light, the BART guidance strongly recommends using CALPUFF for source-receptor distances greater than 50 km but also presents CALPUFF as an option that can be considered for shorter transport distances.

As discussed above, there do not appear to be any scientific reasons why CALPUFF cannot be used for even shorter transport distances than 30 km, though, as long as the scale of the plume is larger than the scale of the output grid so that the maximum concentrations and the width of the plume are adequately represented and so that the sub-grid details of plume structure can be ignored when estimating effects on light extinction. The standard 1-km output grid that has been established for Class I area analyses should serve down to source-receptor distances somewhat under 30 km; how much closer than 30 km will depend on the topography and meteorology of the area and should be evaluated on a case-by-case basis. For extremely short transport distances, depiction of the concentration distribution will require a grid that is finer than 1 km. (For reference, the width of a Gaussian plume, $2\sigma_y$, is roughly 1 km after 10 km of travel distance, assuming Pasquill-Gifford dispersion rates under neutral conditions.)

As an additional consideration, if the plume width is small compared to the visual range, the atmospheric extinction along a typical sight path of tens of kilometers through the plume will be inhomogeneous and the simple CALPOST point estimate of regional light extinction at a receptor point will not be correct. However, the effect of averaging light extinction estimates for 24 hours, during which the plume location shifts over various receptor points, is likely to mitigate this problem to some degree and suggests that using CALPUFF at distances under 30 km will often be appropriate. For the narrow plumes that result from short transport distances, though, the modeled peak 24-hr average extinction at a receptor will tend to overstate the effect of the source on regional haze.

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[5] *Revision to the Guideline on Air Quality Models: Adoption of a Preferred General Purpose (Flat and Complex Terrain) Dispersion Model and Other Revisions; Final Rule.* 70 FR 68218-68261. 9 November 2005.

The U.S. EPA has suggested that the plume visibility model, PLUVUE-II, could be used in lieu of CALPUFF for simulating visibility effects at such short distances.[6] PLUVUE-II is a Gaussian model that simulates the dispersion, chemical conversion, and optical effects of emissions of particles, SO_2, and NO_x from a single source. Its outputs include the discoloration of the sky by the plume (so called "plume blight") and the effect of the plume on visibility along user-selected sight paths that pass through the plume. The impacts of the plume on visibility depend not only on the plume composition, but also on the sight path chosen and its direction relative to the axis of the plume and the location of the sun. It isn't clear how such sight-path dependent results could be compared to the 0.5 and 1.0 deciview thresholds in the BART guidance. Since CALPUFF is designed to be useful for short transport distances (with features such as the simulation of plume downwash caused by structures at the source), CALPUFF seems more appropriate than PLUVUE-II for evaluating source impact at short distances for BART assessment purposes.

3.2.2 Aerosol Constituents

Primary $PM_{2.5}$

Appendix A of the *Guideline on Air Quality Models* (40 CFR 51, Appendix W) states that CALPUFF can treat primary pollutants such as PM_{10}. In actuality, CALPUFF can simulate PM_{10} or $PM_{2.5}$ or some other size range, because the assumed size distribution of the particles is a user input. The smaller the particles, the more they disperse like an inert gas. In most cases, the dispersion of inert $PM_{2.5}$ particles will be only minutely different from that of an inert gas, but the behavior of larger particles will differ.

A particularly important contributor to PM concentrations is the rate of deposition to the surface. $PM_{2.5}$ particles, which have a mass median diameter around 0.5 µm, have an average net deposition velocity of about 1 cm/min (or about 14 m/day) and thus the deposition of fine particles is usually not significant except for ground-level emissions. On the other hand, coarse particles (those PM_{10} particles larger than $PM_{2.5}$) have an average deposition velocity of more than 1 m/min (or 1440 m/day), which is significant, even for emissions from elevated stacks.

CALPUFF includes parametric representations of particle and gas deposition in terms of atmospheric, deposition layer, and vegetation layer "resistances" and, for particles, the gravitational settling speed. Gravitational settling, which is of particular importance for the coarse fraction of PM_{10}, is accounted for in the calculation of the deposition velocity. Effects of inertial impaction (important for the upper part of the PM_{10} distribution) and Brownian motion (important for small, sub-micron particles) and wet scavenging are also addressed. The BART guidance recommends that fine particulate matter (less than 2.5 µm diameter), which has higher light extinction efficiency than coarse particulate matter (2.5-10 µm diameters), should be treated separately in the model. CALPUFF allows for user-specified size categories to be treated as

[6] However, for the reasons given in this paragraph, VISTAS does not recommend PLUVUE-II for BART application

separate species, which includes calculating size-specific dry deposition velocities for each size category.

A primary $PM_{2.5}$ emission from coal-fired electric generating units (EGUs) that is of relevance to visibility calculations is that of primary sulfate. Although primary sulfate emissions account for only a small fraction of the total sulfur emissions from such sources, it may be important to simulate their effect with CALPUFF, especially at shorter distances before significant formation of secondary sulfate conversion from SO_2 has taken place.

Sulfur Dioxide and Secondary Particulate Sulfate

The MESOPUFF-II chemistry algorithm used in CALPUFF[7] simulates the gas phase oxidation of sulfur dioxide to sulfate by a linear transformation rate that was developed using regression relationships derived from the analysis of chemical conversion rates produced by a complex photochemical box model (see Scire et al., 1984, for a description of the development of the chemical module). As in all empirically-derived models, the relationships are based on easily-computed or observed parameters that are used as surrogates for the factors that control SO_2 oxidation.

The surrogate factors included in the parameterized chemistry during the daytime hours include solar radiation intensity, ambient ozone concentration, and atmospheric stability class. For example, gas phase SO_2 oxidation is a function of OH radical concentrations. Ozone concentrations are correlated with OH radical concentrations during daytime hours, and their use in the daytime SO_2 conversion rate in CALPUFF is based on this correlation relationship. The philosophy is that OH radical measurements are not available and cannot easily be computed within a model like CALPUFF, but ozone is commonly measured throughout the country, so the use of the well-known surrogate variable (ozone) is more useful in the empirical relationship than factors that are unknown or have a high degree of uncertainty. The same logic applies to the other variables in the relationship. They are surrogates for factors that the regression analysis has shown to be important in SO_2 oxidation rates. At night, the SO_2 conversion is set to a constant low value (default is 0.2%/hr). Aqueous phase oxidation of SO_2 is represented by an additive term that varies with relative humidity and peaks at 3%/hr at 100% relative humidity. CALPUFF represents the chemical conversion as a linear process because it requires linear independence between puffs, although as explained below, non-linear behavior in nitrate formation can be modeled.

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[7] CALPUFF offers two options for parameterizing chemical transformations: the 5 species (SO_2, $SO_4^{=}$, NO_x, HNO_3, and NO_3^-) MESOPUFF-II system and the 6 species RIVAD system (which treats NO and NO_2 separately). IWAQM recommends using the MESOPUFF-II system with CALPUFF. The RIVAD system is believed to be more appropriate for clean environments, however, and therefore was used in the Southwest Wyoming Regional CALPUFF Air Quality Modeling Study in 2001. For the VISTAS region, the IWAQM- and FLM-recommended MESOPUFF-II chemistry is most appropriate.

The IWAQM Phase 2 report concludes that this chemistry algorithm is adequate for representing the gas phase sulfate formation but that it does not adequately account for the aqueous phase oxidation of SO_2. Actual aqueous phase oxidation in clouds or fog can proceed at rates much greater than 3% per hour, leading IWAQM to suggest that sulfate might be underestimated in such situations. However, aqueous phase oxidation depends on liquid water content, not relative humidity. In reality, liquid water does not exist in the atmosphere at relative humidity much below 100%, while the CALPUFF aqueous reaction term produces sulfate at lower relative humidity. This can lead CALPUFF to overestimate sulfate concentrations when the humidity is high but the cloud water that enables aqueous conversion is not present. Therefore, the direction of the bias in the aqueous chemistry simulation of sulfate formation can vary.

Other potential sources of error in the sulfate formation mechanism of CALPUFF include (1) overestimation of sulfate formation when NO_x concentrations in the plume are high and in actuality they deplete the local availability of ozone and hydrogen peroxide for oxidizing the SO_2; and (2) lack of direct consideration of the effect of temperature on the conversion rates, which may cause the model to overstate sulfate formation on cold days (below 10C or 50°F) (Morris et al., 2003). However, in CALPUFF, the effects of temperature are, to some degree, compensated for indirectly by the use of the solar radiation surrogate variable in the empirical conversion equations.

Whether these potential errors are important will depend on the setting. For example, Figure 3-2 shows a comparison of predicted and observed 24-hour sulfate concentrations, due to a large number of SO_2 sources, at the Pinedale IMPROVE site in Wyoming for the 1995 period (Scire et al., 2001). Overall, in this case there was very little bias in the sulfate predictions. Whether CALPUFF predictions would compare as well with measurements in the Southeast remains to be seen.

CALPUFF does not identify the chemical form of the sulfate compound that results from its reactions, which will generally be some form of ammoniated sulfate whose degree of neutralization will depend on the availability of ammonia in the atmosphere. This consideration, which has been found to be relevant for calculating light extinction in the VISTAS region, is not addressed by CALPUFF or CALPOST.

In most applications, the ozone concentrations required for the sulfate formation calculations are derived from ambient measurements, although concentrations simulated by regional models can be used.

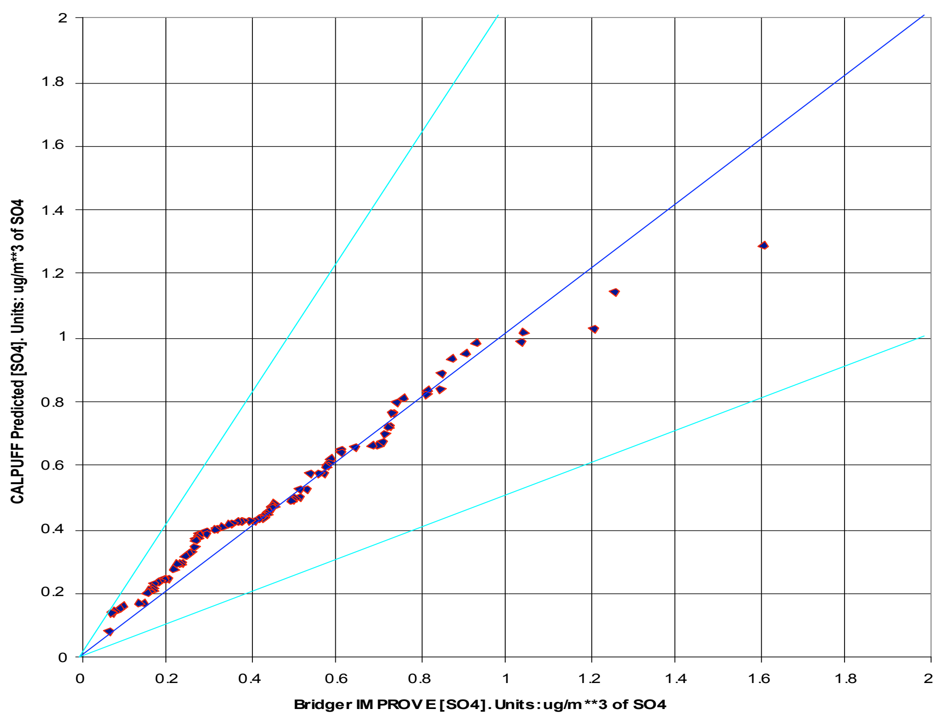

Figure 3-2. Observed vs. CALPUFF-predicted 24-hour sulfate concentrations at the IMPROVE monitoring site in Pinedale, Wyoming for 1995.

NO_x and Secondary Ammonium Nitrate

The MESOPUFF-II chemistry algorithm used in CALPUFF simulates the oxidation of NO_x to nitric acid and organic nitrates (both gases) by transformation rates that depend on NO_x concentration, ambient ozone concentration, and atmospheric stability class during the day. The conversion rate at night is set at to a constant value (default is 2.0 %/hr). The temperature- and humidity-dependent equilibrium between nitric acid gas and ammonium nitrate particles is taken into account when estimating the ammonium nitrate particle concentration, an equilibrium that depends on the ambient concentration of ammonia. The user supplies the value of the ambient concentration of ammonia. CALPUFF assumes that the sulfate reacts preferentially with that ammonia to form ammonium sulfate and the left over ammonia is available to form ammonium nitrate.

The IWAQM Phase 2 report considers that this mechanism is adequate for representing nitrate chemistry. Potential situations where this assumption may not be correct, however, include (1) plumes with high concentrations of NO_x that deplete the ambient ozone and thus limit the transformation of NO_x to nitric acid in the plume; and (2) when ambient temperature is below 10 C, and thus the transformation rate is much slower and the nitrate concentration may be lower than that simulated by CALPUFF (Morris et al., 2003). In both cases, CALPUFF may overestimate the amount of nitrate that is produced. In particular, the impact of ammonium nitrate concentrations on visibility at Class I areas in the VISTAS region is greatest in the winter, when temperatures are lowest, the nitrate concentrations are the greatest, and the sulfate concentrations tend to be the least. CALPUFF may overstate the impacts of NO_x emissions at those times, especially in the colder northern states**.** This potential overestimate of nitrate was not evident, however, in an evaluation of CALPUFF-modeled nitrate against actual observational data in the Wyoming study, as shown in Figure 3-3a (Scire et al., 2001),

Another factor in the calculation of nitrate is that CALPUFF makes the full amount of the background concentration of ammonia available to each puff, and that amount is scavenged by the sulfate in the puff. If puffs overlap, then that approach could overstate the amount of ammonium nitrate that is formed in total if, in reality, the combined scavenging by the overlapping puffs at a location would deplete the available ammonia enough that the combined nitrate formation was limited by the availability of ammonia. This effect of such ammonia limiting can be large in summer; for a source 75 km west of Mammoth Cave National Park, one modeling analysis found the maximum light extinction impact of the source to be 7.4% (roughly 0.74 deciviews) at the park when CALPUFF was used without consideration of ammonia limiting and about 30% less, between 5.5 and 5.8% (roughly 0.55 to 0.58 dv), when the effect of ammonia limiting was considered (Escoffier-Czaja and Scire, 2002).

To address the issue, since 1999 (i.e., after the IWAQM Phase 2 report) the CALPUFF system has included the optional POSTUTIL postprocessing program, which repartitions the ammonia and nitric acid concentrations estimated by CALPUFF to reflect potential ammonia-limiting effects on the development of nitrate**.** This allows non-linearity associated with ammonia limiting effects to be included in the CALPUFF model estimates. POSTUTIL computes the total sulfate concentrations from all sources (modeled sources plus inflow boundary conditions) and estimates the amount of ammonia available for total nitrate formation after the preferential scavenging of ammonia by sulfate. That is, as new sulfate, nitrate or ammonia from the source of interest is added to an existing mix of pollutants, POSTUTIL will estimate both the nitrate formed from the new source and the change in background nitrate as a result of the incremental depletion of ammonia (due to the new sulfate and nitrate) or addition of ammonia (from a new source of ammonia).

Reliable estimates of the ambient concentrations of ammonia, especially with the temporal and spatial resolution that would be optimal for use with CALPUFF, are needed to take full advantage of the increased accuracy provided by POSTUTIL. The processor requires estimated concentrations of ammonia throughout the modeling domain and period. Such estimates can be inferred from CASTNet measurements, which are integrated over a week, from 24-hr SEARCH measurements, or from the output of a regional photochemical model such as CMAQ or CAMx. The CASTNet network is fairly sparse and the uncertainty in the ammonia measurements is large, so defining the ammonia concentration throughout the Southeast would require extensive interpolation or extrapolation from the measured values. The quality of the SEARCH measurements is much better, but there are only 8 sites and they do not cover the entire VISTAS domain. Modeled concentrations have the advantage of being resolved in space and time, but their accuracy should be evaluated by comparison with measurements wherever possible.

Benefit is obtained by considering seasonal trends of ammonia and using POSTUTIL to determine the diurnal variability in available ammonia due to the daily cycle of nitrate formation associated with temperature and relative humidity effects. For example, results of the Wyoming study (see Figure 3-3a) show that POSTUTIL adjustments produced daily average nitrate concentrations well within the factor of two lines and with very little mean bias. On the other hand, analysis of the same results with use of constant ammonia of 0.5 ppb or 1.0 ppb produced consistent overpredictions of nitrate by factors of 2-3 and 3-4, respectively, as shown in Figure 3-3b (Scire et al., 2003).

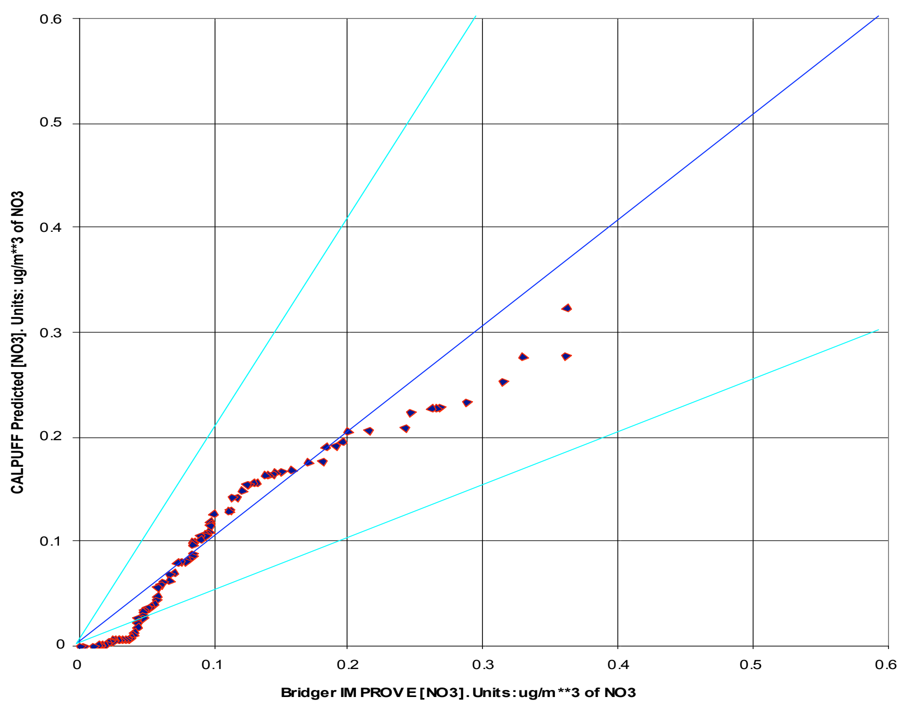

Figure 3-3a. Observed vs. CALPUFF-predicted 24-hour nitrate concentrations at the IMPROVE monitoring site in Pinedale, Wyoming for 1995 using the ammonia limiting method. (Scire et al., 2001)

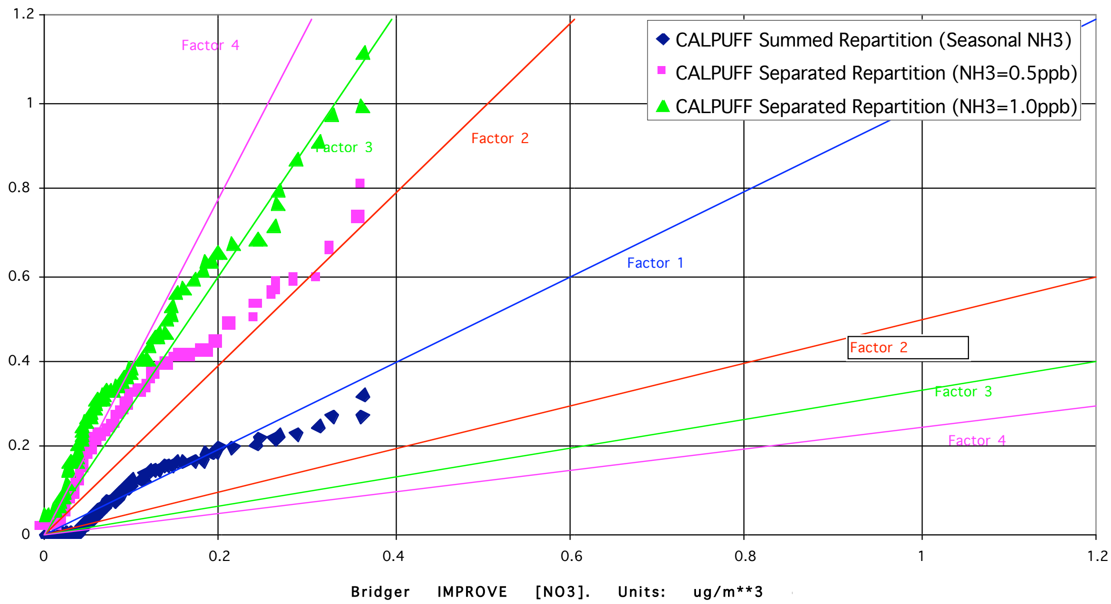

Figure 3-3b. Observed vs. CALPUFF-predicted 24-hour nitrate concentrations at the IMPROVE monitoring site in Pinedale, Wyoming for 1995 using the ammonia limiting method (blue), constant ammonia at 0.5 ppb (pink) and constant ammonia at 1.0 ppb (green). (Scire et al., 2003)

Secondary Organic Aerosol

Ongoing research studies at several Class I areas throughout the country (Fallon and Bench, 2004) and at SEARCH sites in the Southeast (Edgerton et al., 2004) are finding that, typically, 90 to 95% of the rural organic carbon fine particle concentration consists of modern carbon (e.g., that from the burning of vegetation and deriving from VOC emissions from vegetation) and only 5 to 10% is attributable to man's burning of fossil fuels. In addition, a field study at Great Smoky Mountains National Park in August 2002 (Tanner, et al., 2005) found that an average of 83% of the fine carbon was modern carbon

According to IMPROVE measurements, organics account for roughly 10% of the particle-caused light extinction in Class I areas in the Southeast. We can thus conclude that, in general, secondary organic carbon particles derived from anthropogenic fossil fuel burning emissions are unlikely to have a large impact (around 1%) on current visibility. (Man-caused burning of vegetation can have significant localized, short-term impacts, however.)

Current organic fine particle concentrations in the Southeast are typically within a factor of 2 of the 1.4 $\mu g/m^3$ concentration assumed for natural conditions by the EPA, which means that current fossil fuel burning would contribute less than 2% to visibility in an atmosphere that represents natural conditions. Thus, it is unlikely that VOC and organic particle contributions from BART sources will cause a large impact to visibility at Class I areas, but a 5% (0.5 dv) localized impact from a particularly large VOC source cannot be dismissed out of hand.

CALPUFF has only rudimentary capabilities for addressing formation of visibility-impairing organic particles from some forms of volatile organic carbon (VOC). The capabilities that do exist include the following.

First, PM_{10} emissions (such as from power plants) are often divided into filterable and condensable components, with the condensable mass being 100-200% of the filterable mass. For purposes of visibility analyses with CALPUFF, a fraction of the condensable part is typically treated as organic particles, i.e., it is assumed that a fraction of the condensable components in the PM_{10} emissions condense into organic $PM_{2.5}$ particles. The size of this organic fraction varies with process and process equipment, and can range from 20 to 100% of the condensable mass. These fine organic particles can be readily modeled by CALPUFF. (The remaining condensable material may be sulfuric, hydrochloric, or hydrofluoric acid.)

Second, a module that treats the formation of secondary organic particles from organic emissions was recently developed and is now part of the CALPUFF system. (Scire et al., 2001). This simplified secondary organic aerosol (SOA) module is a linear, parameterized representation that is currently considered best suited for biogenic organics. It relies on the conventional wisdom that only hydrocarbons with more than six carbon atoms can form significant SOA (Grosjean and Seinfeld, 1989). For example, according to this rule, isoprene (C_5H_8) does not make SOA but terpenes do, making pine trees more important biogenic contributors to SOA than oak trees.[8]

Limited evaluation of the performance of CALPUFF at simulating SOA with its biogenic SOA module at one IMPROVE site in a regional modeling study in Wyoming found that 95% of 101 estimated 24-hr SOA concentrations were within 2% of the measured values (Scire et al., 2001). This performance seems promising, although the developers view the SOA module as needing more testing and evaluation.

Thus, CALPUFF includes approaches for dealing with condensable VOC emissions that are characterized as condensable PM_{10} and with biogenic VOCs, although the soundness of concentration estimates by these approaches when modeling a plume from a single source is largely untested.[9] The CALPUFF simulation of VOC emissions from sources whose VOC emissions are predominantly anthropogenic is problematic, however. Perhaps the approach used for the simplified biogenic SOA module may be extended to anthropogenic VOCs when speciated VOC emissions information is available. If only those VOCs with more than six carbon atoms are presumed to be of importance, this eliminates many anthropogenic sources of VOC emissions. For example, the fugitive emissions of butane and ethane during petroleum processing

[8] Recent research suggests that isoprene may be a SOA precursor, however.

[9] Note that neither of these VOC-related simulation approaches is described in the current (Version 5) CALPUFF User's Guide dated January 2001. See the Wyoming report referenced above for a description of this module.

are not important, while aromatic emissions (such as of toluene and xylene) are considered by the SOA module's mechanism. Development, testing, and evaluation would be needed before one could rely on such a module for estimating SOA from anthropogenic SOA emissions, though.

Therefore, to demonstrate the visibility impacts of VOC emissions from BART-eligible sources, means other than CALPUFF will be needed. A technical approach using a regional photochemical model to evaluate visibility impacts of VOC emissions is presented in Section 4.1.3. CALPUFF can be used to estimate the contribution from the primary condensable fraction of PM_{10} emissions, though.

3.2.3 Regional Haze

Calculation of the impact of the simulated plume particulate matter component concentrations on light extinction is carried out in the CALPOST postprocessor. The formula used is the usual IMPROVE/EPA formula, which is applied to determine a change in light extinction due to changes in component concentrations. Using the notation of CALPOST, the formula is the following:

$$b_{ext} = 3\,f(RH)\,[(NH_4)_2SO_4] + 3\,f(RH)\,[NH_4NO_3] + 4[OC] + 1[Soil] + \\ + 0.6[Coarse\ Mass] + 10[EC] + b_{Ray} \qquad (3\text{-}1)$$

The concentrations, in square brackets, are in $\mu g/m^3$ and b_{ext} is in units of Mm^{-1}. The Rayleigh scattering term (b_{Ray}) has a default value of 10 Mm^{-1}, as recommended in EPA guidance for tracking reasonable progress (EPA, 2003a).

There are a few important differences in detail and in notation between the CALPOST formula for estimating light extinction (i.e., Equation 3-1) and that of IMPROVE and EPA. First, the *OC* in the formula above represents organic carbonaceous matter (OMC in IMPROVE's notation), which is 1.4 times the *OC* (i.e., organic carbon alone) in the IMPROVE formula. The *EC* above is synonymous with *LAC* in the IMPROVE formula. CALPOST still uses the old IMPROVE *f(RH)* curve, whose values are documented in the December 2000 FLAG report. That curve differs slightly from the *f(RH)* now used by IMPROVE and EPA (as documented in EPA's regional haze guidance documents), mainly at high relative humidity. Also, CALPOST sets the maximum *RH* at 98% by default (although the user can change it), while the EPA's guidance now caps it at 95%.

The haze index (HI) is calculated from the extinction coefficient via the following formula:

$$HI = 10\ln(b_{ext}/10) \qquad (3\text{-}2)$$

where *HI* is in units of deciviews (dv) and b_{ext} is in Mm^{-1}. The impact of a source is determined by comparing HI for estimated natural background conditions with the impact of the source and without the impact of the source.

CALPOST Methods

CALPOST uses Equation 3-1 to calculate the extinction increment due to the source of interest and provides various methods for estimating the background extinction against which the increment is compared in terms of percent or deciviews.

For background extinction, the CALPOST processor contains seven techniques for computing the change in light extinction due to a source or group of sources (called Methods 1-7). These are usually reported as 24-hour average values, consistent with EPA and FLM guidance. In addition, there are two techniques for computing the 24-hour average change in extinction (i.e., as the ratio of 24-hour average extinctions, or as the average of 24-hour ratios). A brief summary of the techniques is provided below. Method 2 is the current default, recommended by both IWAQM (EPA, 1998) and FLAG (2000) for refined analyses. Method 6 is recommended by EPA's BART guidance (70 FR 39162).

Methods 4 and 5 use optically measured hourly background extinctions, which represent current actual levels of extinction and thus are not consistent with the "natural conditions" the BART proposal says should be used as a baseline. Methods 1 through 3 and 6 and 7 allow for user inputs of estimated (e.g., natural conditions) background extinction or component concentrations, and thus are consistent with the BART proposal.

Method 1 allows the user to specify a single value of a "dry" background extinction coefficient for each receptor, specify that a certain fraction of that coefficient is due to hygroscopic species, and use relative humidity measurements to vary the extinction hourly via a 1993 IWAQM *f(RH)* curve or, optionally, the EPA regional haze f(RH) curve (EPA, 2003b). The *RH* is capped at 98% or a user-selected value (95% for the EPA curve). The same *f(RH)* is applied to both the modeled sulfate and nitrate.

For an example of the use of Method 1, one could use the dry particle extinction coefficient of 9.09 Mm^{-1} that results from EPA's default natural conditions concentrations, together with an assumption that for natural conditions, say, 0.9 Mm^{-1} (or 10%) of this amount results from hygroscopic ammonium sulfate and ammonium nitrate, and then apply *f(RH)* to this 10%.

In Method 2, user-specified, speciated monthly concentration values are used to describe the background. When applied to natural conditions, for which EPA's default natural conditions concentrations are annual averages, the same component concentrations would have to be used throughout the year (unless potential refinements to those default values resulted in concentrations that vary during the year). Hourly background extinction is then calculated using these concentrations and hourly, site-specific *f(RH)* from a 1993 IWAQM curve (a different one than that in Method 1) or, optionally, the EPA regional haze f(RH) curve.[10] Again the *RH* is capped at either 98% (default) or a user-selected value (most commonly at 95%).

Method 3 is the same as Method 2, except that any hour in which the RH exceeds 98% (or the selected maximum) is dropped from the analysis. When 24-hr extinction is computed, no fewer than 6 valid hours are accepted at each receptor; otherwise the value for the day is tabulated as "missing".

Method 6 is similar to Method 2, except monthly f(RH) values (e.g., EPA's monthly climatologically representative values in EPA (2003a, b)) are used in place of hourly values for calculating both the extinction impact of the source emissions and the background conditions extinction. Hourly source impacts, with the effect on extinction due to sulfates and nitrates calculated using the monthly-average relative humidity in f(RH), are compared against the monthly default natural background concentrations. Thus the monthly-averaged relative humidity is applied to the hygroscopic components (i.e., sulfate and nitrate) of both the source impact and the background extinction with Method 6**.**

Method 7 is a new variant of Method 2 that was developed as a result of a ruling by the Assistant Secretary of the Interior for Fish and Wildlife and Parks, in response to a New Source Review case in Montana, that "natural conditions" should reflect the visibility impairment caused by significant meteorological events such as fog, precipitation, or naturally occurring haze (DOI, 2003).[11] Under Method 7, during hours when visibility is obscured by meteorological conditions, the actual measured visibility is used to represent natural conditions instead of the value that is calculated from EPA's default natural conditions concentrations under Method 2. A recent modification developed in response to FLM comments on Method 7, in which the daily average natural extinction is calculated somewhat differently, is called Method 7', i.e., "7 prime".

Refined Estimates of Extinction and Natural Background Visibility

Separate from the BART discussions, IMPROVE, EPA, and the Regional Planning Organizations are evaluating whether refinements are warranted to the methods recommended in EPA's guidance to calculate default estimates of natural background visibility. In addition, IMPROVE has recently approved an alternative to the formula (Eq. 3-1) it uses to estimate extinction from particle concentration measurements (Pitchford et al., 2005).

Refinements in the revised IMPROVE formula include the following:

- Adding a sea salt term, including a growth factor due to relative humidity

[10] Note that the hourly-varying natural background extinction in this method is not consistent with that prescribed by the EPA's natural conditions guidance (EPA, 2003b), for which a "climatologically-representative" f(RH) that only varies monthly is to be used. Method 6 uses these monthly average humidity values.

[11] The Secretary's guidance applies only to Federal Land Managers. EPA's position on this interpretation of natural conditions is unknown.

- Increasing the factor used to calculate the mass of particulate organic matter (OC in Eq. 3-1) from organic carbon measurements

- Modifying the relative humidity growth formula, f(RH), for sulfates and nitrates

- Revising the extinction efficiencies (the numerical constants in Equation 3-1) for sulfates, nitrates, and organic carbon so that they vary with concentration

- Adding a site-specific Rayleigh scattering term to the formula. Values will be calculated by IMPROVE for all Class I areas.

For the purposes of calculating current, future, and natural background visibility at VISTAS Class I areas as part of the reasonable progress analyses, VISTAS intends to present regional air quality modeling results using both the current EPA recommended assumptions and the newly revised aerosol extinction formula. If a BART-eligible source chooses to consider its projected impacts using the newly revised formula as well as the current formula, then modifications would need to be made to CALPOST to carry out calculations with the new algorithm.

4. VISTAS' COMMON MODELING PROTOCOL

4.1 Overview of Common Modeling Approach

In this section, guidance is provided on the use of the CALPUFF modeling system for two purposes:

1) Evaluating whether a BART-eligible source is exempt from BART controls because it is not reasonably expected to cause or contribute to impairment of visibility in Class I areas, and

2) Quantifying the visibility benefits of BART control options.

For purpose 1), States must determine whether a source emits any air pollutant (SO_2, NO_x, PM, and in certain cases VOC and NH_3) that "may reasonably be anticipated to cause or contribute to any impairment of visibility" in a Class I area. The States have 3 options to accomplish this:

A) Conclude that all BART-eligible sources in State are subject to BART.

B) Demonstrate that all BART-eligible sources in the State together do not cause or contribute to any visibility impairment

C) Determine if the impact from each individual BART-eligible source is greater than a threshold value.

VISTAS States intend to follow Option C (determine if the visibility impact from individual sources exceeds a contribution threshold) for SO_2, NO_x, and PM emissions. The methods for Option C are described in Section 4.1.1. Option B (demonstrate that all BART eligible sources in a State do not impact visibility) is being pursued for VOC and NH_3 emissions, and potentially for PM emissions. Methods for Option B are described in Section 4.1.3.

4.1.1 BART Exemption Analysis

As illustrated in Figure 4-1, three steps will evaluate whether a BART-eligible source of SO_2, NO_x, or PM is subject to BART:

1) VISTAS plans to use Q/d as a presumptive indicator that a source is subject to BART. If Q/d for $SO_2 > 10$ for 2002 actual emissions, then the State presumes that the source is subject to BART. If the source agrees with this presumption, then no exemption modeling is required and the source can proceed to the BART determination using CALPUFF to evaluate impacts of control options and can perform the engineering analyses. If a source disagrees, the source may perform fine grid modeling as described in Section 4.4 to determine if its impact is < 0.5 dv.

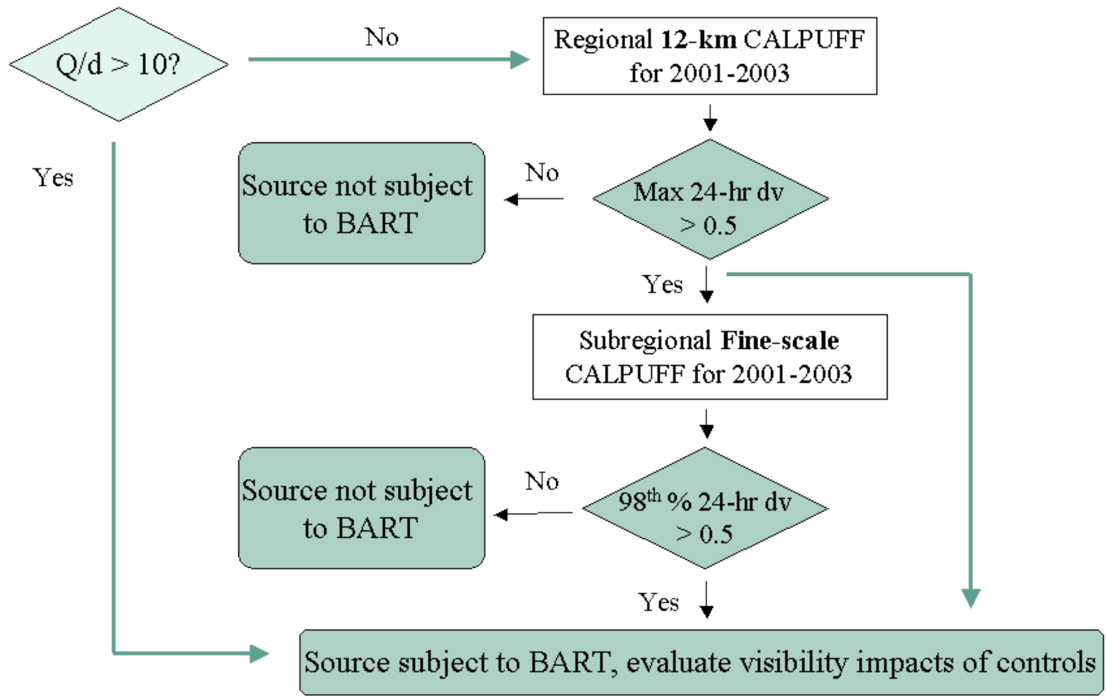

Figure 4-1. Flow chart showing the components of the VISTAS common modeling protocol. Assessment should be made for each Class I Area. (If a source agrees to install the most stringent controls then the modeling steps indicated above and engineering analyses and visibility impact modeling would not be required.)

2) An optional initial modeling assessment using the CALPUFF model with the coarse scale 12-km regional VISTAS domain can be used to answer questions whether (a) a particular source may be exempted from further BART analyses and (b) if finer grid CALPUFF analysis were to be undertaken, which Class I areas should be included. Assumptions for the initial modeling assessment are conservative so that a source that contributes to visibility impairment is not exempted in error. If a source is shown not to contribute to visibility impairment using the initial modeling assessment, the source would not be subject to BART and would be exempted from further BART analyses. If a source is shown to contribute to visibility impairment using the initial modeling assessment, the source has the option to undertake finer grid CALPUFF modeling to evaluate further whether it is subject to BART.

3) A finer grid CALPUFF modeling analysis using a subregional CALMET domain will be the definitive test as to whether a source is subject to BART.

For large sources that will clearly exceed the initial screening thresholds, this step can be skipped and the analysis may proceed directly to the finer grid modeling analysis, which is described in Section 4.4.

4.1.2 BART Control Evaluation

For sources that are determined to be subject to BART controls, part of the BART review process involves evaluating the visibility benefits of different BART control measures. These benefits will be determined by making additional CALPUFF simulations using the same CALMET and CALPUFF configuration as those used in the finer grid analysis of Step 2. The only exception is that the source and emissions data used in the CALPUFF control evaluation simulations will reflect the BART control measures being evaluated. Using the same model configuration will produce an "apples-to-apples" comparison, where differences in impacts are due to the effectiveness of the controls rather than model configuration differences. For example, a control scenario evaluation that uses more conservative assumptions than the base case simulation may produce results showing no or little improvement in visibility impacts. That control scenario run with the same model configuration as the base case may show significant visibility improvement. Therefore, in order to not obscure the response to predicted visibility improvements by differences in the modeling approach, the same model configuration should be used in the BART control evaluation simulation as in the base case simulation.

The base case to which the effectiveness of BART controls is to be compared is the "current emissions" scenario for which the finer grid Step 2 modeling was performed. The postprocessing steps and procedures are the same as in the BART eligibility simulation. Side-by-side comparison of the visibility impacts will be tabulated to quantify the effectiveness of each control scenario relative to the base case.

The modeling evaluation is a unit-by-unit evaluation and can be conducted on a pollutant specific basis. Modeling results are used with the other four statutory factors mentioned in Section 2.1 to decide which control technology, if any, is appropriate. Finally, if a source decides to use the most stringent control technology available, the BART control analysis, including modeling, is not necessary.

4.1.3 VISTAS' Treatment of VOC, NH_3, and PM

Volatile Organic Compounds

CALPUFF is currently not recommended for addressing visibility impacts from VOC because its capability to simulate secondary organic aerosol formation from VOC emissions is not adequately tested, especially for anthropogenic emissions. (Separately, condensable organic carbon can be calculated from PM_{10}.)

VISTAS is currently performing a weight of evidence analysis to demonstrate, using the CMAQ regional air quality model, that all VOC emissions from all point sources (BART-eligible and non-BART) in each State do not contribute to visibility impairment. Emissions sensitivity simulations run for VISTAS by Georgia Institute of Technology using VISTAS' 12 x 12 km grid and CMAQ v 4.3 for episodes in July 2001 and January 2002 demonstrated very low to no response of organic carbon levels and light extinction at Class I areas to changing VOC emissions from all anthropogenic sources in the VISTAS 12-km modeling domain (eastern US). Georgia Tech is currently repeating the sensitivity analyses for VISTAS using the VISTAS 12-km domain and CMAQ v 4.4 with a refined SOA module for a summer (Jun 1-Jul 10) and winter (Nov 19-Dec 19) period in 2002. VOC emissions from all anthropogenic point sources in each VISTAS State are being reduced. Given that the impact of eliminating all VOC emissions from all point sources in a State is less than 0.5 dv, then the impact of any one BART-eligible source would be less than 0.5 dv. Based on these analyses, the VISTAS States have concluded that VOC emissions should not be subject to BART. When similar analyses for NH_3 and PM have been completed, a technical justification for treatment of all three of these pollutants will be presented to EPA and FLMs for their review.

Ammonia

EPA has given states the option to address ammonia (NH_3) emissions from BART-eligible sources. VISTAS has also contracted with Georgia Tech to perform emissions sensitivities using CMAQ v 4.4 with a refined SOA module and the Jun-Jul and Nov-Dec periods in 2002. All NH_3 emissions from point sources (BART-eligible and not-BART) in each State are reduced for these analyses. If the sensitivity evaluation shows that the collective impact of all point NH_3 emissions is less than 0.5 dv, then the impact of a single BART eligible source would be less than 0.5 dv. In that case, the VISTAS States would recommend that NH_3 emissions not be subject to BART.

Primary Particulate Matter

Primary particulate matter is considered a visibility impairing pollutant. However, the extent to which primary PM from BART-eligible sources contributes to impairment at Class I areas in the southeastern US is not clear. For EGUs, the EPA has determined that emissions reductions of SO_2 and NO_x under the CAIR rule meet the BART requirements, but these EGUs may still be subject to BART for primary PM. To determine the potential impacts of PM from EGU and non-EGU sources in the VISTAS states, two CMAQ sensitivity runs are underway for the first and third quarters of 2002. In one run, all primary PM from EGUs is removed while in the other run all primary PM from non-EGU sources is removed. All other CMAQ modeling components are held constant. The results will help determine at which, if any, Class I areas in the VISTAS region primary PM emissions contribute to regional haze. If the sensitivity evaluation shows that the collective impact of all EGU or non-EGU point primary PM emissions is less than 0.5 dv, then the impact of primary PM from any single BART eligible source would necessarily be less than 0.5 dv. These results will be reported at the same time as results for VOC and NH_3.

4.2 Optional Source-Specific Modeling

In some circumstances, a source may want to apply techniques designed to evaluate the impacts in a more detailed way than the standard VISTAS common protocol. A source may propose source-specific modeling procedures to address special issues to the State for State review. For example, sources very close to Class I areas may be better treated by a finer grid resolution that the generic Step 2 “fine” grid resolution meteorological fields provided by VISTAS. In some situations, higher resolution MM5 or other prognostic meteorological datasets may be available than the standard 12-km or 36-km MM5 datasets provided by VISTAS. Because it is not possible to anticipate all of the situations where there would be a benefit to conducting more detailed source-specific analyses, the option to pursue this option is left as an open issue, to be resolved and justified based on specific factors relevant for the source in question.

A source-specific modeling protocol is required for each source. This document should describe the data sources and model configuration, and provide rationale for any changes in the model approach from the common protocol. This source-specific protocol must be provided for review and approval by the State. The State will share the protocol with EPA and the Federal Land Managers for their review. Discussion of approaches to source-specific modeling and an outline of the typical contents of the source-specific protocol are presented in Chapter 5. Discussions with the regulatory authorities should be conducted prior to development of a source-specific protocol to ensure all of the relevant issues are included in the protocol.

4.3 Initial Procedure for BART Exemption

4.3.1 Overview of Initial Approach

The first step in the common protocol, the initial assessment in Figure 4-1, is a simple procedure to evaluate whether a source can be exempted from BART controls using a consistent set of meteorological and dispersion options. A pre-computed set of meteorological files and a pre-defined CALPUFF input option configuration, based on guidance in the final BART rule (70 FR 39104-39172) and other EPA and FLAG model guidance, will allow relatively simple initial simulations. The regional initial domain is designed to allow any Class I areas within the VISTAS area to be evaluated with a single meteorological database and consistent CALPUFF modeling options. The second important question that this first screening step will answer is, if initial modeling indicates a source may impact visibility significantly, what Class I areas should be included in a finer grid analysis? Due to the multitude of factors affecting the contribution of a source to visibility in a Class I area, simple screens or rules of thumb alone (such as that the closest Class I area will produce the controlling visibility impacts) are not likely to be universally reliable.

4.3.2 Discussion of 12-km Initial Exemption Modeling

Meteorological Fields

A regional initial domain and a set of pre-computed regional CALMET meteorological files will be prepared for VISTAS, to allow any Class I areas within the VISTAS area to be evaluated with a consistent meteorological database and consistent CALPUFF modeling options.

The following three years of MM5 meteorological data have been assembled by VISTAS for use in the regional CALPUFF modeling effort:

- 2001 MM5 dataset at 12 km and 36 km grid (developed for EPA)

- 2002 MM5 dataset at 12 km and 36 km grid (developed by VISTAS)

- 2003 MM5 dataset at 36 km grid (developed by the Midwest Regional Planning Organization).

These data sets have been provided to Earth Tech by VISTAS, and from them Earth Tech has produced annual CALMET meteorological files at 12-km grid resolution for the domain shown in Figure 4-2. The CALMET modeling output files in the form of CALPUFF-ready three-dimensional meteorological files will be available on external hard drives to the States and other parties.

The initial procedure to determine if a BART-eligible source is subject to BART uses the pre-computed CALMET meteorological fields for the years 2001-2003 on the 12-km CALMET domain in Figure 4-2 and simulates with CALPUFF any BART-eligible source to be screened. The CALMET simulations will be developed using the highest resolution MM5 data available for each year (i.e., 36-km MM5 data for 2003, 12-km MM5 data for 2001 and 2002).

The development of the regional CALMET meteorological fields from MM5 data will be conducted in No-Observations ("No-Obs") mode. The MM5 data already reflect assimilation of observational data and are likely to adequately characterize regional wind patterns that are consistent with the 12-km grid scale. Blending of MM5 data with local observations (which are mainly at the surface) could lead to wind structures that may not be realistic under some conditions and may result in poorer characterization of the regional winds. Thus, the effort required to prepare observational data sets for CALMET for the large regional domain involves considerable effort that may not provide corresponding improvement of the wind field.

For 2003, the 36-km MM5 data will be used as CALMET's initial guess field and then the CALMET diagnostic terrain adjustments (see Section 3.1.1) will be applied to reflect terrain on the scale of the CALMET grid (i.e., 12-km). When the 12-km MM5 (2001 and 2002) data are used, the diagnostic CALMET terrain adjustments will be turned off since the grid resolution of the MM5 data is the same as the CALMET grid and the terrain adjustments on the 12-km grid scale will already be reflected in the MM5 dataset. In this case, the MM5 winds will be interpolated by CALMET to the CALMET layers and CALMET's boundary layer modules will compute mixing heights, turbulence parameters and other meteorological parameters that are required by CALPUFF.

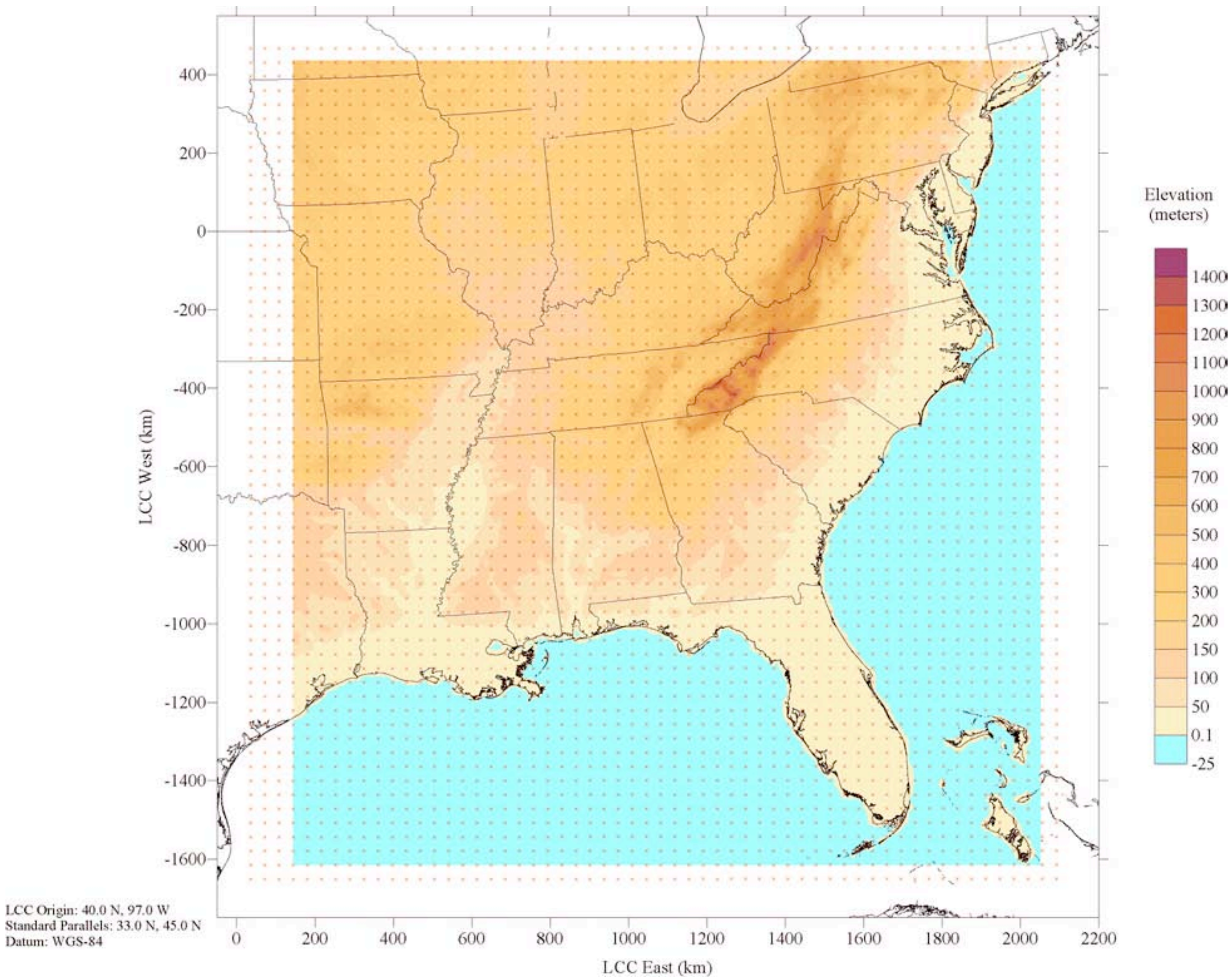

Figure 4-2. VISTAS Regional 12-km Resolution CALMET Modeling Domain (color area with terrain contours). The locations of the 36-km resolution MM5 grid points are shown on the plot.

Impact Threshold

The final BART guidance recommends that the threshold value to define whether a source "contributes" to visibility impairment is 0.5 dv change from natural conditions (although states may set a lower threshold). The 98^{th} percentile (8^{th} highest annual) 24-hr average predicted impact at the Class I area, as calculated using CALPOST Method 6 (monthly average relative humidity values), is to be compared to this contribution threshold value. For this comparison, the predicted impact at the Class I area on any day is taken to be the highest 24-hr average impact at any receptor in the Class I area on that day. (Note that the receptor where the highest impact occurs can change from day to day.) According to clarification of the BART guidance received from EPA, for a three-year simulation the modeling values to be compared with the threshold are the greatest of the three annual 8^{th} highest values or the 22^{nd} highest value over all three years combined, whichever is greater.

For the purposes of the initial analysis, however, the *highest value* over the three-year period (not the 98^{th} percentile value) is to be compared to the contribution threshold. This ensures a significant measure of conservatism in the initial approach. VISTAS will evaluate the initial CALPUFF results to determine if using the single highest value provides too conservative a screen for exemption purposes. If so, VISTAS may increase the number of exceedances of the contribution threshold that would be allowed and still qualify to exempt a source.

4.3.3 Model Configuration and Settings for Initial Analysis

VISTAS will use CALPUFF Version 5.754 and CALMET Version 5.7. These versions contain enhancements funded by the Minerals Management Service (MMS) and VISTAS. They were developed by Earth Tech, Inc. and they are maintained on Earth Tech's Atmospheric Studies Group CALPUFF website (www.src.com) for public access. This version includes CALMET, CALPUFF, CALPOST, CALSUM, and POSTUTIL as well as CALVIEW.

The initial analysis uses a CALPUFF computational domain that includes all Class I areas within 300 km of a source. These Class I areas are specified in the CALPUFF control file for analysis. States could decide to require a different value for the maximum distance threshold for the CALPUFF domain, depending on the locations of the Class I areas in their states and other factors such as meteorological conditions and the magnitudes of the emissions from BART-eligible sources. The regional CALMET domain will be unchanged by these adjustments.

Also, the initial approach is designed to significantly reduce the CALPUFF simulation time by restricting the CALPUFF computational domain size to include only areas where significant impacts are feasible rather than the entire regional domain. CALPUFF allows its computational domain to be specified as a subset of the CALMET meteorological domain by settings within the CALPUFF input file. The advantage of selecting a smaller CALPUFF computational domain in the regional CALPUFF simulations is that CALPUFF run time is proportional to the number and residence time of the puffs on the domain (and other factors such as the number of receptors and the internal time step computed by the model). A CALPUFF domain covering an area 300 km from a source in all directions would involve only 50 x 50 12-km grid cells, which will require modest computational resources.

CALMET output files for the VISTAS regional domain shown in Figure 4-2 will be provided to VISTAS by Earth Tech. These files will be in CALPUFF-ready format, and as such, no CALMET user inputs will be required. An option in CALMET allows finer grid CALMET input files to be calculated from the 12-km CALMET files.

The basic characteristics of the CALMET, CALPUFF and CALPOST configurations for the initial analyses are listed below.

CALMET Modeling Configuration (12-km initial exemption modeling)

The CALMET model configuration for the regional CALMET simulations will be defined by Earth Tech in collaboration with the VISTAS States. The basic model configuration will follow the recommended IWAQM guidance (EPA, 1998; Pages A-1 through A-6), except as noted below.

The basic features of the modeling simulation are the following:

- Modeling period: 3 years (2001-2003)

- Meteorological inputs: MM5 data provide initial guess fields in CALMET

- CALMET grid resolution: 12-km (same Lambert Conformal coordinate system and grid cells as the 12-km 2001/2002 MM5 simulations)

- CALMET vertical layers: 10 layers. Cell face heights (meters): 0, 20, 40, 80, 160, 320, 640, 1200, 2000, 3000, 4000.

- CALMET mode: No-Observations mode including option to read overwater data directly from MM5.

- Diagnostic options: IWAQM default values, except as follows: diagnostic terrain blocking and slope flow algorithms used for 2003 simulations (using 36-km MM5 data), but no diagnostic terrain adjustments in 2001 and 2002 simulation (using 12-km MM5 data)

- CALMET options dealing with radius of influence parameters (R1, R2, RMAX1, RMAX2, RMAX3), BIAS, ICALM parameters are not used in No-Observations mode.

- TERRAD (terrain scale) is required for runs with diagnostic terrain adjustments (i.e., the 2003 simulations). Values of ~10-20 km will be tested, and an appropriate value determined.

- Land use defining water: JWAT1 = 55, JWAT2 = 55 (large bodies of water). This feature allows the temperature field over large bodies of water such as the Atlantic Ocean and the Great lakes to be properly characterized by buoy observations.

- Mixing height averaging parameter (MNMDAV) will be determined by Earth Tech for the regional simulations based on sensitivity tests. The purpose of the testing is to optimize the variable to allow spatial variability in the mixing height field, but without excessive noise.

- Geophysical data for regional runs: SRTM-GTOPO30 30-arcsec terrain data, Composite Theme Grid (CTG) USGS 200m land use dataset. References for these and other CALMET datasets can be found on the CALPUFF data page of the official CALPUFF site (www.src.com).

CALPUFF Modeling Configuration (Initial exemption modeling)

The CALPUFF model configuration for the regional CALPUFF initial simulations will follow the recommended IWAQM guidance (EPA, 1998; Pages B-1 through B-8), except as noted below:

- CALPUFF domain configured to include the source and all Class I areas within 300km of the source plus 50km buffer zone in each direction. CALPUFF is recommended for all source-receptor distances to be considered in the BART analyses.

- Chemical mechanism: MESOPUFF II module

- Background concentrations of SO_4 and TNO_3 (HNO_3 + NO_3) from CMAQ 2001-2003 annual runs

- Species modeled: SO_2, SO_4, NO_x, HNO_3, NO_3 and particulate matter in size categories of <0.625 µm, 0.625-1.0 µm, 1.0-1.25 µm, 1.25-2.5 µm, 2.5-6.0 µm and 6-10 µm aerodynamic diameters. As noted below, the particulate matter emissions by size category will be combined into the appropriate species for the visibility analysis (i.e., elemental carbon (EC), fine PM or "soil" (< 2.5 µm in diameter), coarse PM (between 2.5-10 µm in diameter) and organics (called secondary organic aerosols (SOA) in the CALPOST postprocessor).

- Emission rates for modeling based on EPA BART guidance, i.e., maximum 24-hour actual emission rate with normal operations from the highest emitting day of the meteorological period modeled (excluding days where start-up, shutdown or malfunctions occurred sometime during the day.) Note that potential emissions are used to determine if a source is BART-eligible, but 24-hour average maximum emissions are used for modeling purposes (70 FR 39162). Pollutants considered include SO_2, H_2SO_4, NO_x and PM_{10}.

Condensable emissions are considered as primary fine particulate matter and allocated equally to the two submicrometer particle size classes. If actual source emissions data are not available, the modeling should be based on permit limits. If source-specific size categories are not available, then AP-42 factors may be used for sources where AP-42 factors are available. For sources where AP-42 factors are not available, assumptions for partitioning will be investigated by VISTAS based on review of available source categories.

Excluded from the modeling are pollutants with plant-wide emissions less than *de minimis* levels (40 tons per year for SO_2 and NO_x and 15 tons per year for PM_{10}). *De minimis* levels are plant wide for each visibility-impairing pollutant, so individual units may be modeled even if they have emissions below *de minimis* if the plant total is greater than *de minimis*.

- Particulate emissions speciation: Break down, as appropriate, filterable and condensable particulate matter into the following species categories: elemental carbon (soot), "soil" (fine

PM < 2.5 µm diameter), coarse particulate matter (2.5-10 µm diameter) and organics. The process is illustrated in Figure 4-3. If source-specific emissions factors are not available, AP-42 factors can be used to estimate the PM speciation for those source sectors for which AP-42 emissions factors have been developed. Otherwise assumptions will need to be proposed by the source, and reviewed and approved by the state.

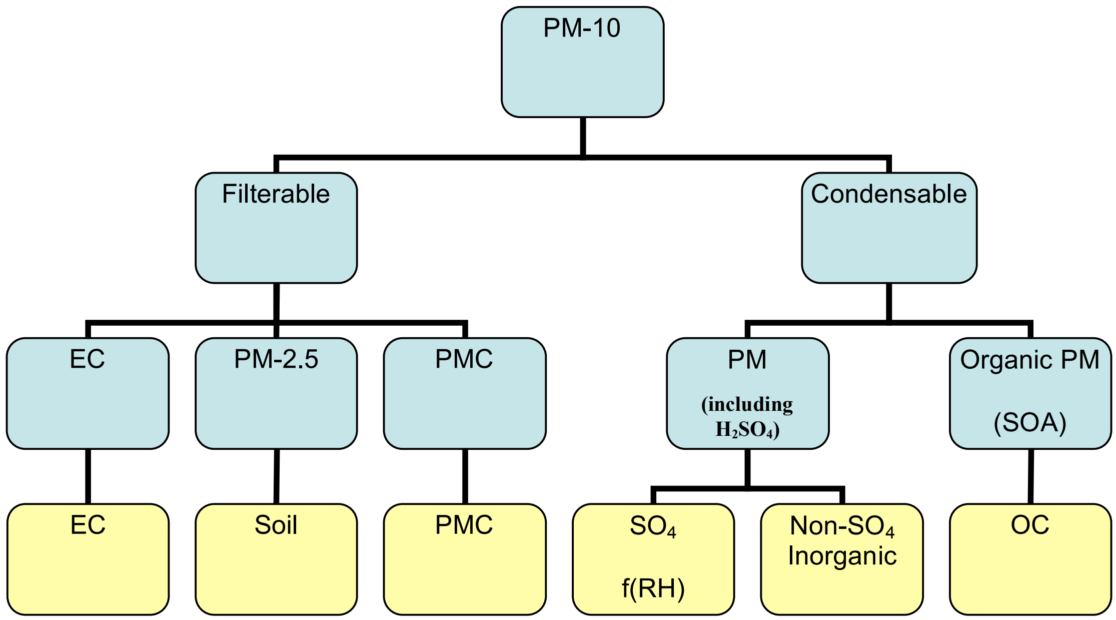

Figure 4-3. Speciation of PM-10 Emissions. (PMC is coarse particulate matter -- 2.5 to 10 µm diameter.)

- Class I receptors: Use FLM Class I receptor list with receptor elevations provided (available from the NPS).

- CALPUFF model options: Use IWAQM (EPA, 1998) default guidance, including Pasquill-Gifford dispersion coefficients.

- Ozone dataset – use observed ozone data for 2001-2003 from CASTNet and AIRS stations. Only non-urban ozone stations should be used in the OZONE.DAT file. Monthly average ozone (backup) background values are to be computed based on daytime average ozone concentrations from the OZONE.DAT file (6am-6pm average ozone concentrations computed by month).

- Background ammonia concentration: In CALPUFF, use constant (0.5 ppb) values for ammonia.

- Puff representation: integrated puff sampling methodology.

- Building downwash: Ignore building downwash unless source is within 50-km of a Class I area and the State instructs the source to specifically consider building downwash.

CALPOST and POSTUTIL Configuration (Initial exemption modeling)

- Use Visibility Method 6 (for initial modeling), with EPA (2003a, b) Class I area-specific (centroid) monthly relative humidity values

- Species considered in visibility analysis: SO_4, NO_3, EC, SOA (i.e., condensable organic emissions), soil, coarse PM

- Natural background light extinction: Method 6 requires input of natural background concentrations while the EPA provides (EPA, 2003b) haze index value (in deciviews) for the 20% best days. To produce the appropriate natural background in CALPOST, use Equation 3-2 to calculate the extinction coefficient that corresponds to EPA's haze index value for the Class I area, subtract the Rayleigh scattering value of 10 Mm^{-1}, and enter a soil concentration (in $\mu g/m^{3)}$ into CALPOST that is numerically equal to this result. (Since the extinction efficiency of soil is 1 m^2/g, Equation 3-1 shows that this produces a background extinction that equals the EPA's value.)

- Light extinction efficiencies: Use EPA (2003a) values. If a source chooses, the new IMPROVE algorithm for calculating light extinction (see Section 3.2.3) may be used in addition to the default IMPROVE algorithm. (Calculations would need to be performed outside CALPOST or CALPOST would need to be modified to accommodate the new algorithm.)

- Ammonia Limiting Method: Do not use for the initial modeling.

The initial run results will be based on the highest change in light extinction (deciviews) from natural conditions over the three-year modeling period for each Class I area considered. Predicted changes exceeding the "contribution" threshold (0.5 deciviews) will trigger a finer grid CALPUFF modeling analysis.

4.4 Finer Grid Modeling Procedures

4.4.1 Rationale for and Overview of Finer Grid Modeling Approach

There are two potential applications for finer grid CALPUFF modeling:

BART Exclusion Modeling. First, finer grid CALPUFF modeling can be used to demonstrate that a source does not cause or contribute to visibility impairment in any Class I areas, and thus can be excluded from BART controls. As shown in Figure 4-1, if the initial regional modeling results are not below the threshold for visibility impacts, the next step is to conduct modeling using a finer grid resolution for the meteorological fields and the treatment of terrain effects and land use variability. In the finer grid modeling the predicted visibility impairment that is compared to the threshold is based on the BART guidance of the 98th percentile change in deciviews value rather than the more conservative highest value used in the initial analysis.

The BART guidance indicates that the emissions rate to be used for such modeling is the highest 24-hr rate during the modeling period. Depending on the availability of source data, the following emissions information (listed in order of priority) should be used with CALPUFF for BART exclusion modeling:

- 24 hr maximum value emissions for the period 2001-2003 (Continuous Emission Monitor, CEM data)
- 24 hr maximum value from continuous emissions monitoring data
- facility stack test emissions
- potential to emit
- permit allowable emissions, if available
- emissions factors from AP-42 source profiles

Quantify Benefits of BART. The second application of refined modeling is to quantify the visibility benefits from the BART control options. This is accomplished by running CALPUFF with the baseline emissions rates and again with emissions after BART controls. It is important that emission reductions be evaluated in the postprocessing step rather than by using "negative" emission rates in the CALPUFF model. The chemical scheme requires that emission rates always be positive.

For any of these applications, a source-specific modeling protocol that defines source properties and the specific model configuration is required. As discussed in Section 5, the source specific protocol should include source-specific emissions data and can refer to this document for all methods and assumptions that follow this common protocol.

4.4.2 Model Configuration and Settings for Finer Grid Modeling

Grid resolution substantially better than 12-km is needed for a finer grid CALPUFF assessment of visibility impacts in most cases involving Class I areas in complex terrain or coastal areas. Thus, the CALMET fine grid resolution in the subregional modeling domains used for finer grid modeling will depend on the terrain, land use (especially coastal boundaries), location of the source, distance of the source from Class I areas, and total size of the subregional modeling domain.

VISTAS intends to provide 2001-2003 CALMET files for five 4-km sub-regional domains as illustrated in Figure 4-4. The subdomains are designed to address all BART eligible sources within each VISTAS states and all Class I areas within 300 km of the BART-eligible sources. For application for a single source, a smaller domain of roughly 200-300 km by 200-300 km is recommended.

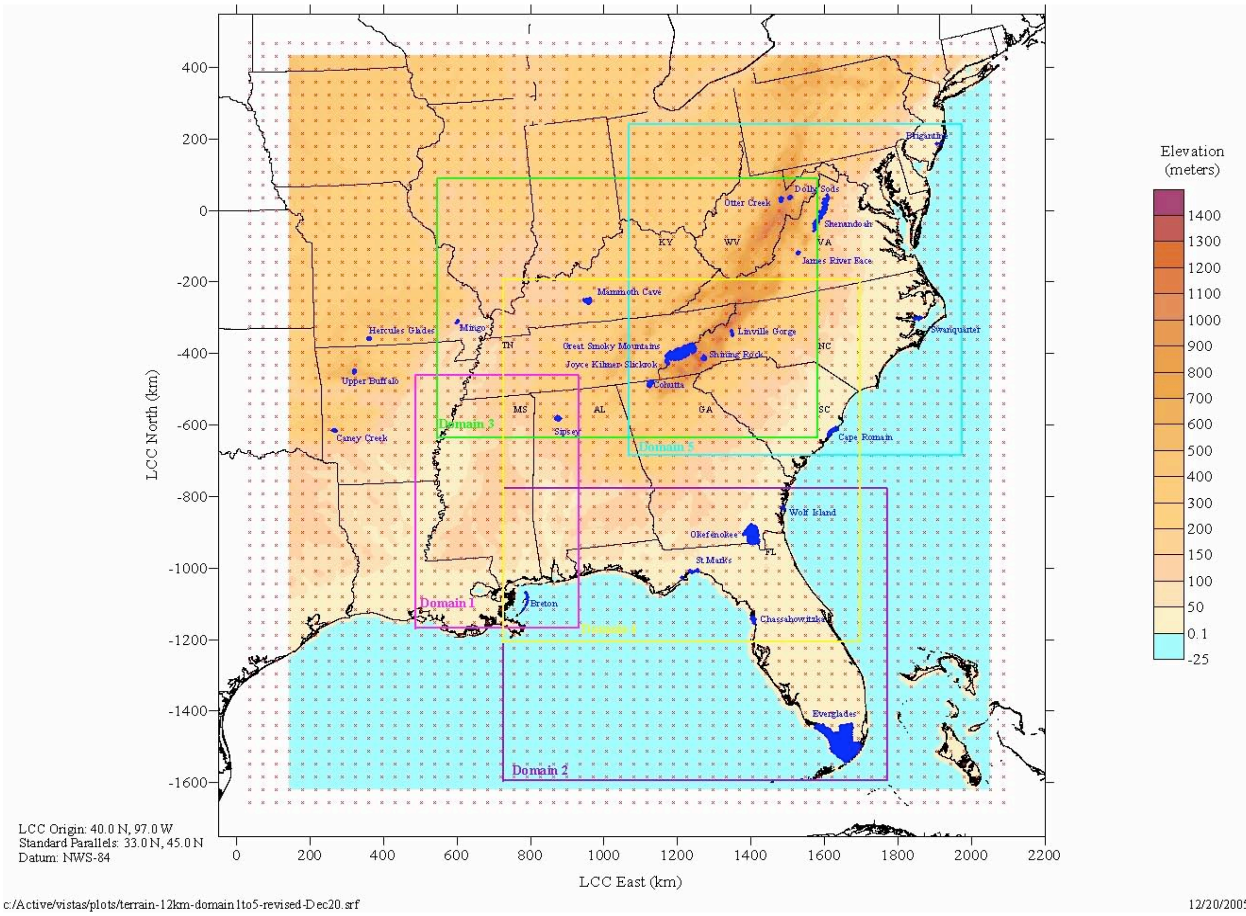

Figure 4-4. The five subregional domains for 4-km CALMET modeling.

In some instances, as part of the source-specific protocol, a source may propose to the State to use an even finer grid simulation to properly characterize the flow fields and land use changes that affect dispersion. An application for source-receptor distances within about 50 km may require a grid resolution less than 1 km if complex terrain effects are likely to be important. This determination should be made on a case-by-case basis. There is not a single distance at which a particular grid size is appropriate. It depends on factors such as the complexity of the terrain, the source-receptor distances involved, the location of the source relative to the terrain features, the physical stack parameters (e.g., a tall stack in complex terrain may be unaffected by the terrain-forced flow), proximity of the source and Class I area to a coastline, and other factors including availability of representative observational data.

The finer grid CALMET simulations will be run by Earth Tech in hybrid mode, using both MM5 data to define the initial guess fields and meteorological observational data in the Step 2 calculations. Overwater (buoy) data will be provided in addition to the hourly surface meteorological observations, precipitation observations and twice-daily upper air sounding data.

A domain-specific set of modeling parameters will be defined for each subregional domain. The proper selection of the CALMET diagnostic wind field parameters that are used to blend observations with the Step 1 wind field depends on factors such as the locations of the meteorological stations relative to terrain and coastal features (which affects the representativeness of the observational data), the terrain length scale, and the quality (resolution) of the MM5 data used to define the initial guess field and its ability to properly resolve wind flows on the fine-scale CALMET domain. The definition of the proper CALMET parameters is done as part of sensitivity testing where model performance is evaluated against available observations and expected terrain effects, such as channeling of flows within a valley.

In addition to the better grid resolution and the introduction of observational data in the finer grid simulations, several other modeling refinements can enhance the accuracy of the finer grid modeling. These include use of the higher resolution terrain DEM data (~3 arc sec USGS data) in defining the gridded terrain fields and application of the ammonia limiting method in the POSTUTIL post-processor (using Class I area specific monthly diurnal profiles of NH_3 concentrations developed from the 2002 CMAQ regional modeling performed by VISTAS). Otherwise, the source configuration, emissions, pollutant speciation, Class I receptors, ozone datasets and CALPUFF model options will be the same as in the initial runs.

For the finer grid BART exclusion analysis, the test for evaluating whether a source is contributing to visibility impairment is based on the 98th percentile modeled value (rather than the highest predicted value used for the initial evaluation), which is consistent with EPA's BART guidance. A coding change is required in the CALPOST postprocessor in order to allow the 98th percentile change in extinction to be computed.

4.5 Presentation of Modeling Results

The CALPOST processing computes the daily maximum change in deciviews. A sample of the summary table produced by CALPOST is shown in Table 4-1. For evaluating compliance with the VISTAS screening threshold, the highest change in extinction value, located at the bottom of the CALPOST list file is compared to the threshold value (e.g., 0.5 dv). For example, in the sample shown in Table 4-1, the summary at the bottom shows that the highest visibility impact is 1.219 dv, with 9 days over the year showing values greater than 0.5 dv. Therefore this source would not pass the initial analysis, and finer grid modeling would be required.

Table 4-1. Example of CALPOST Output, Showing Maximum Daily Impacts of Source and Locations of Those Impacts.

YEAR	DAY	HR	RECEPTOR	COORDINATES (km)		TYPE	DV(Total)	DV(BKG)	DELTA DV	F(RH)	%_SO4	%_NO3	%_OC	%_EC	%_PMC	%_PMF
2001	2	0	3	20.540	79.782	D	5.397	5.358	0.039	4.314	44.33	47.22	3.07	1.07	0.00	4.30
2001	3	0	9	31.680	79.822	D	4.566	4.421	0.145	1.767	40.75	33.89	9.19	3.24	0.00	12.94
2001	4	0	1	24.723	77.951	D	4.540	4.540	0.000	2.076	0.00	0.00	0.00	0.00	0.00	0.00
2001	5	0	77	30.228	94.571	D	4.950	4.939	0.011	3.144	43.13	44.74	4.64	1.45	0.00	6.05
2001	6	0	1	24.723	77.951	D	5.181	5.166	0.015	3.772	38.58	56.05	1.90	0.70	0.00	2.76
2001	7	0	3	20.540	79.782	D	6.366	5.745	0.620	5.439	44.98	44.99	3.69	1.26	0.00	5.08
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2001	363	0	113	27.414	103.782	D	5.725	5.652	0.073	5.164	53.49	35.51	4.03	1.39	0.00	5.58
2001	364	0	113	27.414	103.782	D	6.554	6.521	0.033	7.826	48.12	47.09	1.67	0.64	0.00	2.48
2001	365	0	1	24.723	77.951	D	6.499	6.499	0.000	7.757	0.00	0.00	0.00	0.00	0.00	0.00

```
--- Number of days with Delta-Deciview  =>   0.50:         9
--- Number of days with Delta-Deciview  =>   1.00:         2
---             Largest Delta-Deciview  =             1.219
```

In addition to the highest change in deciview value on each day over all the receptors in a particular Class I area, the CALPOST summary table in Table 4-1 contains the coordinates of the receptor, receptor type (D indicates discrete receptors), the total haze level (background + source, in dv), the background haze in deciviews, the change in haziness (delta dv), the humidity term applied to hygroscopic aerosols (F(RH)), and the contribution of each species to light extinction (in percent of the total source contribution) for SO_4, NO_3, organics, elemental carbon, coarse and fine particulate matter.

For the finer grid analysis, the data in the table can be imported into a spreadsheet and sorted on the delta dv column. Table 4-2 shows an example of the ranked visibility impacts (change in dv) for each of three years at six different Class I areas. The 98th percentile (8th highest value) in the sorted table would be compared to the contribution threshold (e.g., 0.5 dv). In the example shown in this table, the source passes the finer grid analysis because the highest 98th percentile visibility impact is below the contribution threshold of 0.5 dv.

The Results section of the CALPUFF modeling report should contain the following information:

1. Map of source location and Class I areas within 300 km of the source

2. For the VISTAS 12-km CALPUFF initial exemption modeling domain, a table listing all Class I areas in the VISTAS domain and those in neighboring states and impacts at those Class I areas within 300 km of the source, as illustrated in Table 4-3**.**

3. A discussion of the number of Class I areas with visibility impairment from the source on 98th percentile days in each year greater than 0.5 dv (total visibility impairment minus impairment on 20% best days for natural background visibility equals delta-dv, the visibility impact attributed to the source).

4. For the Class I area with the maximum impact, discussion of the number of days below the 98th percentile that the impact of the source exceeds 0.5 dv, the number of receptors in the Class I area where the impact exceeds 0.5 dv, and the maximum impact.

5. For finer grid CALPUFF exemption modeling, results for those Class I areas for which impacts of the source exceeded 0.5 dv in the 12-km initial exemption modeling. Report same results as provided for 12-km initial exemption modeling.

6. For control option modeling, each control option tested should be listed in tabular format. For each control option and for each Class I area where the impact of the source exceeded 0.5 dv, report the change in pollutant emissions and the change in visibility impact from the source as a result of the control option. The effectiveness of candidate control options are to be compared to each other, not to a specific target improvement.

Table 4-2. Example of Visibility Impact Rankings at Six Class I Areas

Class I Area	2001	2002	2003
	Delta-Deciview Ranks 1-8	Delta-Deciview Ranks 1-8	Delta-Deciview Ranks 1-8
Great Smoky NP	0.99	0.95	1.20
	0.88	0.63	0.90
	0.62	0.51	0.73
	0.59	0.50	0.72
	0.55	0.46	0.59
	0.52	0.42	0.47
	0.48	0.37	0.45
	0.47	0.36	0.42
Linville Gorge	0.67	0.81	0.76
	0.45	0.69	0.47
	0.43	0.65	0.37
	0.33	0.50	0.35
	0.29	0.45	0.31
	0.27	0.33	0.30
	0.25	0.31	0.28
	0.23	0.29	0.28
Shining Rock	0.66	0.73	0.75
	0.43	0.69	0.45
	0.41	0.63	0.36
	0.35	0.52	0.34
	0.26	0.46	0.28
	0.24	0.34	0.27
	0.23	0.29	0.26
	0.22	0.26	0.25
Cohutta	0.26	0.54	0.61
	0.23	0.47	0.42
	0.22	0.43	0.30
	0.21	0.37	0.29
	0.20	0.37	0.28
	0.19	0.31	0.28
	0.18	0.31	0.25
	0.16	0.30	0.25
Joyce Kilmer-Slickrock	0.34	0.52	0.27
	0.33	0.43	0.24
	0.31	0.32	0.23
	0.26	0.31	0.20
	0.24	0.30	0.14
	0.20	0.28	0.13
	0.18	0.24	0.11
	0.17	0.24	0.10
Mammoth Cave NP	0.56	0.57	0.50
	0.44	0.56	0.37
	0.38	0.53	0.36
	0.29	0.35	0.35
	0.25	0.33	0.31
	0.24	0.33	0.24
	0.22	0.30	0.21
	0.21	0.29	0.19

Table 4-3. Format of Summary of Results for CALPUFF Modeling in VISTAS' 12-km Modeling Domain to Determine if a BART Eligible Source is Subject to BART.

Class I area	Distance (km) from source to Class I area boundary	# of days[1] and # of receptors with impact > 0.5 dv in Class I area: 2001		# of days[1] and # of receptors with impact > 0.5 dv in Class I area: 2002		# of days[1] and # of receptors with impact > 0.5 dv in Class I area: 2003		# of days[1] and # of receptors with impact > 1.0 dv in Class I area for 3-yr period		Max. 24-hr impact over 3-yr period
Dolly Sods, WV										
Shenandoah, VA										
James River Face, VA										
Mammoth Cave, KY										
Sipsey, AL										
Great Smoky Mtns, TN										
Cohutta, GA										
Shining Rock, NC										
Linville Gorge, NC										
Swanquarter, NC										
Cape Romain, SC										
Okefenokee, GA										
Saint Marks, FL										
Chassahowitzka, FL										
Everglades, FL										
Brigantine, NJ										
Breton Island, LA										
Caney Creek, AR										
Upper Buffalo, AR										
Mingo, MO										
Hercules Glade, MO										

[1]Days below the 98^{th} percentile of days in each year or the three-year modeling period, as appropriate

States will provide further guidance on graphic presentation of results to simplify evaluation of effectiveness of control measures. For example, a temporal plot of the change in deciviews between the controlled and uncontrolled cases could be developed for the receptor with the maximum modeled impact in each Class I area.

7. Copies of all input files and input data in electronic format for the CALMET, CALPUFF, CALPOST and POSTUTIL runs should be archived and provided to the State.

4.6 VISTAS Contribution to CALPUFF Modeling of BART Eligible Sources

VISTAS will provide updates and supporting information concerning the Common Modeling Protocol (this document) on the VISTAS website. In addition, VISTAS will make publicly available the following data bases developed by Earth Tech:

- VISTAS version of the CALPUFF modeling system, maintained on the Earth Tech website. Version 5.754 includes CALMET, CALPUFF, CALPOST, and POSTUTIL files, updated in December 2005. The last update in this VISTAS version is a CALMET update that addresses over water dispersion, which was developed for Mineral Management Services (MMS) in fall 2005. When available in January 2006, this VISTAS version of CALPUFF will not be updated further unless errors are found in the code. BART-eligible sources in the VISTAS states will be able to use this VISTAS version throughout the BART modeling exercise.

- 12-km CALMET output files for 2001, 2002, and 2003 produced as described in previous sections. Further detail on model configuration and settings will be provided with the output files and will be made available on the CALPUFF website.

- CALMET will include a software modification to allow the meteorological data inputs into CALMET to be used to generate finer grid CALMET files without having to go back to the original MM5 output files

- Five 4-km CALMET subdomains for 2001, 2002, and 2003, produced as described in previous sections. Further detail on model configuration and settings will be provided with the output files and will be made available on the website.

- File with CALPUFF model configuration and settings sufficient to replicate CALPUFF modeling done for VISTAS using 12 km CALMET, including
    - Ozone data used to run CALPUFF
    - Ammonia data used to run CALPUFF and to partition NO_3 in POSTUTIL.
    - Background concentrations files for use in POSTUTIL
    - All other set up files used in VISTAS 12-km CALPUFF run

5. SOURCE-SPECIFIC MODELING PROTOCOL

Sources are required to submit a source-specific protocol to the State for review and approval prior to source-specific modeling. States will provide the documentation to EPA and FLM for their review. An outline of the typical contents of the site-specific protocol is provided in Table 5-1.

If a source-specific modeling approach is proposed that differs from the common approach in Chapter 4, a more-detailed modeling protocol than that required under the common procedures is required. This protocol must explain the data sources, model configuration, and rationale for changes in the model approach from the common protocol and must be approved by the State.

Unit-specific source data include the following parameters:

- Location (e.g., UTM coordinates, UTM zone and datum)
- Stack height above the ground
- Stack diameter
- Exit velocity
- Exit temperature
- Emission rates (SO_2, H_2SO_4, NO_x and PM_{10}).

Additional building dimension information (building width, length, height and corner locations) is needed for short stacks that are less than Good Engineering Practice (GEP) height. This information is used in providing effective structure dimensions for building downwash calculations. (The requirement to conduct building downwash modeling may be waived by individual States or if the transport distance is greater than 50 km.)

The source coordinates must be expressed in the coordinate system used to define the CALMET and CALPUFF modeling domains. For the regional screening simulations, a Lambert Conformal Conic (LCC) coordinate system will be used. The required parameters to define an LCC coordinate include two matching parallels, latitude/longitude of the projection origin, coordinate datum, and false Easting and Northing (if used) of the projection origin. Subregional and source-specific domains may be using either an LCC or UTM projection.

The Earth Tech Graphical User Interface (GUI) system provides software (called COORDS) to compute to/from latitude/longitude, LCC and UTM coordinates for a large number of datums. In addition, the CALVIEW graphics feature allows the use of georeferenced satellite or aerial photographs to be used as base maps to confirm source locations. Links to sources of suitable base maps can be found on the CALPUFF data site (www.src.com) in the section on "Aerial Photos".

Table 5-1. Sample Table of Contents of a Source-Specific Fine-Scale Modeling Protocol.

An example of the data that need to be reported is provided in Table 5-2. More detail on the stack data, emissions species, and particulate size fractions to be reported will be made available on the VISTAS website, www.src.com, Check with your State for the more detailed format of Table 5-2 that is to be used.

Discussions with the regulatory authorities should be conducted prior to development of a protocol to ensure all of the relevant issues are included in the protocol.

Table 5-2. Example of Source Documentation for BART Eligible Source.

Unit name and/or description	**Start-up dates**	**SO_2 potential emissions (tpy)**	**NO_x potential emissions (tpy)**	**Total PM potential emissions (tpy)**
Emissions source name				
…				
Total emissions				
Potential BART-eligible emissions				

6. QUALITY ASSURANCE

6.1 Scope and Purpose of the QA program

Air quality modeling covered under this protocol is an important tool for use in determining whether a BART-eligible source can be reasonable expected to cause or contribute to visibility impairment in a Class I area, and therefore whether this source should be subject to BART controls, and if so, to determine the relative benefits of various BART controls. The purpose of the quality assurance (QA) program is to establish procedures for ensuring that products produced by the application of the modeling techniques for BART studies satisfy the regulatory objectives of the BART program.

The scope of the QA program affects different users differently. Common features of most applications will be the setup and execution of the CALPUFF air quality model and processing of modeling results to determine if a source contributes to visibility impairment at a Class I area. In many cases, users will be provided meteorological datasets that have been developed with VISTAS funding under a suitable QA program for use in the BART modeling. Other users will be involved in site-specific or source-specific analyses that will use additional datasets and potentially different modeling options and/or tools. More extensive quality assurance will be required in these latter types of applications. It is the responsibility of the modeler to ensure that an adequate QA protocol is in place for a particular application.

The CALPUFF modeling system contains built-in features to facilitate quality assurance of the modeling results. These include the automatic production of “QA” files for various datasets, including geophysical fields, sources and receptors, and imbedded tracking of model options and switches within the output files from the major modeling units of the modeling system. The Graphical User Interface system (GUI) provided as part of the latest CALPUFF modeling system allows these QA files to be displayed graphically.

In addition, a detailed software management system is in place to track version and level numbers associated each program and utility within the CALPUFF modeling system. This information is carried forward in all of the output files to create an audit trail of software versions and major model options used that can be retrieved and displayed from the model output files.

Because the required QA procedures will depend heavily on the exact application, there will be differences among different users and different applications.

In addition, the BART modeling process involves multiple organizations. The States have overall responsibility for the process and may also execute some or all of the modeling. VISTAS is contributing general guidance via this protocol and is preparing meteorological fields and performing modeling under the guidance of the States. The sources that are BART-eligible need to provide process information and emissions data for use in the analyses. In addition, those sources that are involved in BART assessments will need to be actively involved in control technology decisions and assessments. Finally, some of the modeling steps may be carried out by contractors on behalf of VISTAS, a State, or a source.

Each of these organizations has a responsibility to ensure that it is providing correct information to others and to evaluate the quality of any analyses it is performing, whether with data of its own or from others. This chapter provides general guidance and information on those aspects of quality assurance that are specific to the CALPUFF modeling effort, irrespective of which organization is carrying out the effort. The focus is on the common protocol efforts described in Chapter 4. As described in Section 6.3, more comprehensive QA may be needed for the unique aspects of the source-specific modeling described in Chapter 5.

6.2 QA Procedures for Common Protocol Modeling

The VISTAS common protocol (Section 4) describes the methods and procedures for use in conducting regional scale screening modeling to determine the whether a particular source or group of sources is subject to BART controls. In the initial application, the regional CALPUFF-ready meteorological data files will be provided by VISTAS. The amount of effort for end-users performing QA of these pre-defined meteorological fields will be reduced from what is required in developing source-specific meteorological fields, as described below. Also, VISTAS is planning to provide five subregional CALMET meteorological datasets in a CALPUFF-ready format. The development of these CALMET datasets will be subject to a QA program as part of their development, so the necessary quality assurance activity of end-users is again reduced from what would be required in the development of the dataset. It is not expected that the quality assurance steps in the development will be repeated in each application. The VISTAS-provided regional and subregional meteorological fields will include a test case simulation for demonstrating that expected modeling results are obtained on the user's computer platform. This test should be repeated by every user.

Although the CALPUFF modeling system is recommended by the U.S. Environmental Protection Agency for application to BART analyses, a considerable amount of expertise and modeling judgment is needed at certain stages of the analysis. The modeling is not a "cookbook" exercise, a fact that was recognized by the U.S. EPA in describing the expertise needed for CALMET modeling (EPA, 1998; pp. 9-10,). Current methods for performing refined chemistry calculation also require an understanding of the chemical and meteorological processing affecting ammonium nitrate formation. VISTAS has committed to provide appropriate CALPUFF training to assist States in obtaining the necessary expertise with the latest CALPUFF modeling tools and techniques. An appropriate level of knowledge of the model formulation, technical approach and assumptions is essential for successful BART modeling.

6.2.1 Quality Control of Input Data

The input data required by the model depends on the application. At a minimum, source data is required by CALPUFF (see Section 6.2.3) along with a list of choices made about model options and switches. Most of the modeling option choices are specified or recommended by regulatory guidance and default values (see references in Section 4.3.3). However, remodeling of the boundary conditions is not required for VISTAS-provided finer grid domains so the expertise level is not as high as it would be for development of the boundary conditions files from scratch.

To the extent that modeling applications are using pre-defined CALMET files and CALPUFF templates, the quality assurance will be straightforward. More detailed steps are needed for the setup of modeling files for source-specific applications of subregional domains finer than 4 km.

The basic procedures that will apply to all CALPUFF model applications will include a confirmation of the source data, including units, verification of the correct source and receptor locations, including datum and projection, confirmation of the switch selections relative to modeling guidance, checks of the program switches and file names for the various processing steps, and confirmation of the use of the proper version and level of each model program. It is a common and recommended procedure for an independent modeler not involved in the setup of the modeling files to independently confirm the model switches and data entry in the actual model input files and to conduct an independent run of the worst case event as a confirmation check.

In addition, common practice requires that a model project CD (or DVD or set of DVDs) be created that contains all of the data and program files needed to reproduce the model results presented in a report. The model list files from each step are included on the project CD. This information allows independent checking and confirmation of the modeling process.

6.2.2 Quality Control of Application of CALMET

For users of the VISTAS CALPUFF-ready CALMET meteorological files, a number of large datafiles will be provided by VISTAS on external USB2 or Firewire hard drives in a format ready for use with the CALPUFF model. The QA steps associated with the development of the VISTAS common datasets will be provided separately as part of the modeling documentation. It is not expected that the QA steps conducted in the development of the meteorological datasets will be repeated in each application, although tests to confirm that the dataset is suitable for the application for which it is being used should be performed as part of the QA. This is discussed in more detail below.

The regional screening CALMET grid is defined in Chapter 4 on a 12-km Lambert Conformal Conic (LCC) grid system. The subregional and source-specific domains may be defined in either LCC or Universal Transverse Mercator (UTM) coordinates. In the case of the LCC projection, two matching parallels, latitude/longitude of the projection origin, coordinate datum, and false Easting and Northing (if used) of the projection origin must also be defined. For any domains in UTM coordinates, the UTM zone (see Appendix D of the CALMET User's Guide) and datum must be defined. The appropriate projection and map factors are provided as part of the definition of the VISTAS regional grid system. For a source-specific domain, the grid parameters will be provided as part of the source-specific protocol.

Appendix A of the IWAQM report (EPA, 1998) contains a list of recommended CALMET switch settings. Except as modified in Chapter 4 of this protocol or in a source-specific protocol, the IWAQM guidance should be used in setting up the CALMET simulations. The CALMET model obtains the switch settings from an ASCII "control file" with a default name of CALMET.INP. Whether the model is run using a GUI or from the control line in a DOS, Linux, or Unix window, it is essential that the control file be reviewed as part of the CALMET QA analysis. The CALMET GUI retains all of the input descriptive information that is part of the standard CALPUFF.INP file structure. This includes the default value for each variable, a text description of the variable, the meaning of each variable option, the units of the variable and inter-relationships among variables indicating if/when the variable is used. Some third-party commercial GUIs strip out this descriptive information, which makes the QA step more difficult, although it is essential for perform nonetheless using the variable names as references for the variables in the file.

Part of the CALPUFF modeling system's built-in QA capabilities is a variable tracking system that retains the control file inputs for CALMET and CALPUFF in the output files create by the models. This information includes the Version and Level numbers of the processor codes and main model codes used in the simulations as well as the control files from the main models (CALMET and CALPUFF). The information from the preprocessing steps and the CALMET and CALPUFF model simulations is all carried forward and saved in the CALPUFF/postprocessor output files so that the final concentration/flux files contain a history of the model options and switch settings. This allows a user or reviewing agency to confirm the switch settings provided in a control file with that actually used in the model simulations. An optional switch in the CALPOST processor creates a complete listing of the QA data. This step requires access to the output CALPUFF concentration and/or flux files, which are normally practical to store on CDs or DVDs and to provide a part of the Project CD/DVD set.

6.2.3 Quality Control of Application of CALPUFF

The quality assurance of the source and emissions data is a major component of the CALPUFF modeling. Also, many errors are found in source coordinates and related projection/datum parameters, so confirmation of the source location is an important part of the modeling QA.

The locations of the Class I area receptors are another important CALPUFF input. The use of pre-defined receptors as provided by the National Park Service (NPS) receptor dataset is recommended in the VISTAS common protocol. However, although the latitude and longitude of each receptor point is provided, it is necessary to ensure that the proper UTM or LCC coordinates have been computed for computational domain selected. In particular, the datum of the NPS conversion software is not specified, so it is recommended that coordinates be checked using the CALPUFF GUI's COORDS software or another comparable coordinate translation software package that recognizes various datums.

Most of the CALPUFF input variables contain default values. Appendix B of the IWAQM report contains a list of recommended CALPUFF switch settings. Except as modified in Chapter 4 of this protocol or in a source-specific protocol, the IWAQM guidance should be used in setting up the CALPUFF simulations. The CALPUFF model obtains the switch settings from an ASCII "control file" with a default name called the CALPUFF.INP file. As is the case with the comparable CALMET file, it is essential that the control file be reviewed manually as part of the CALPUFF QA analysis. To facilitate this process, as was the case with the CALMET GUI, the CALPUFF GUI retains all of the input descriptive information that is part of the standard CALPUFF.INP file structure. Some third-party commercial GUIs strip out this descriptive information, which makes the QA step more difficult, although it is essential for perform nonetheless using the variable names as references for the variables in the file.

6.2.4 Quality Control of Application of CALPOST and POSTUTIL

CALPOST is run separately for each Class I area in order to obtain the necessary visibility statistics for evaluating compliance with the BART screening and finer grid modeling thresholds. The inputs to CALPOST involve selection of the visibility method (Method 6 in the standard EPA BART guidance), entry of Class I area-specific data for computing background extinction and monthly relative humidity factors for hygroscopic aerosols. CALPOST contains a receptor screening that allow subsets of a receptor network modeling in CALPUFF to be selected for processing in a given CALPOST run. This is how receptors within a single Class I area are selected for processing from a CALPUFF output file that may contain receptors from several Class I areas. CALPOST contains options for creating plot files that will help in the confirmation that the proper receptor subset is extracted.

The CALPOST output file contains a listing of the highest visibility impact each day of the model simulation over all receptors included in CALPOST analysis. Receptors will normally be selected in each CALPOST run so that each CALPOST run represents the impacts at a single Class I area. The table includes the data shown in the example in Table 4-1. For a screening assessment, the peak value of the change in extinction is shown at the bottom of the visibility table (see Table 4-1). For a finer grid simulation, the 98th percentile value (8th highest day) is used for comparison against the BART threshold of 0.5 deciviews. It is necessary to import the results of the CALPOST table into a sorting program such as a spreadsheet to rank the daily change in extinction values such as is presented in Table 4-2.

The CALPOST inputs that need to be carefully checked as part of the CALPOST quality assurance are:

- Visibility technique (Method 6 in the common VISTAS protocol)

- Monthly Class I-specific relative humidity factors for Method 6

- Background light extinction values

- Inclusion of all appropriate species from modeled sources (e.g., sulfate, nitrate, organics, (as SOA), coarse and fine particulate matter and elemental carbon.

- Appropriate species names for coarse PM used

- Extinction efficiencies for each species

- Appropriate Rayleigh scattering term (10 Mm^{-1} for screening modeling but Class I area specific value for finer grid modeling)

- Screen to select appropriate Class I receptors for each CALPOST simulation.

The CALPOST program produces plot files compatible with CALVIEW that allow confirmation of receptor locations that is useful in evaluating the receptor screening step.

POSTUTIL allows the user to sum the contributions of sources from different CALPUFF simulations into a total concentration file. In addition, it contains options to scale the concentrations from different modeled species (e.g., different particle sizes) into species-dependent size distributions for the particulate matter. For example, PM is often simulated with unit emission rates for each particle size category and, in the POSTUTIL stage, the contributions of each size category based on the species being considered (e.g., elemental carbon, coarse particulate matter, etc.) are combined to form the species concentrations for input into CALPOST. This process, although simple, requires a careful review of the weighting factors for each source. POSTUTIL also allows a repartitioning of nitric acid and nitrate to account for the effects of ammonia limiting conditions.

If source-specific modeling is performed using different sources of data or different techniques, the source-specific modeling protocol should provide justification for deviations from the VISTAS common protocol, and a QA plan specific for the application provided to address the quality assurance of the data used.

6.3 Additional QA Issues for Alternative Source-Specific Modeling

The level of QA required for application of source-specific protocols will be substantially higher than for the use of datasets that have already been subject to a QA procedure. For example, source-specific protocols may include the use of on-site meteorological datasets, the use of higher resolution prognostic meteorological (e.g., MM5) datasets, alternative visibility calculations, different extinction coefficients, or other changes to the common protocol. In addition to providing a source-specific modeling protocol describing and justifying the changes to the modeling approach from the VISTAS common protocol, the site-specific applications should include the development of a QA plan to properly evaluate the data used in the site-specific modeling.

The critical CALMET input parameters depend on the mode in which the model is run (observations mode, hybrid mode or no-observations mode), and the location and spatial representativeness of any observational data. In a site specific protocol involving the development of a meteorological dataset, the elements of the QA process include preparation of wind rose (using observed, MM5 and CALMET-derived data), including examination of the data as a function of season and time of day (e.g., 4am, 10am, 4pm wind roses), time series analyses, and presentation of 2-D vector plots illustrating terrain effects/sea breeze circulation or other features of the flow expected to occur within the domain. For example, 2-D vector plots produced during light wind speed stable conditions (e.g., early morning such as 4 am) are good for assessing the performance of the CALMET model configuration and switches in reproducing terrain effects because these conditions are likely to maximize the terrain impacts in the model. Season wind roses at 4 am, 10 am and 4 pm would be expected to show the development of sea breeze circulations that may be important for certain applications. Customization of the QA process for the individual site-specific domain based on the availability of data and the physical processes expected to be important at that location should be conducted as part of the site-specific QA plan development.

If site-specific CALPUFF simulations involving the Ammonia Limiting Method are conducted, performance of the model in reproducing observed CASTNet or IMPROVE sulfate and nitrate concentrations at measurement sites within the site-specific modeling domain should be evaluated. The use of alternative ammonia concentration data (e.g., CMAQ output rather than derived ammonia based on aerosol measurements) will require an evaluation of the model performance relative to the techniques in the VISTAS common protocol.

In any site-specific protocol a site-specific QA plan should be prepared.

6.4 Assessment of Uncertainty in Modeling Results

Chapter 3 discussed the uncertainties and known limitations in CALPUFF. The source specific modeling report does not need to repeat the uncertainties listed in Chapter 3, but the reviewer should interpret results in light of these limitations. It is expected that the performance of the model will be better in predicting changes in visibility impacts due to BART controls than in predicting absolute visibility values. This is because uncertainties in meteorological conditions transport and dispersion are expected to be less important in evaluating a change in impact, since a comparable effect will be included in both the base and sensitivity simulations.

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